

Quotients of Group Algebrae in the Calculation of Intermediate Ligand Field Matrix Elements

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The structure of the classes of symmetry elements excluded during the subduction of the representations of $SU(2)$ onto the finite group O^* is shown to quantitatively define the relationship of the coupling algebrae of these two groups. This relationship is formalized as a quotient algebra. This quotient algebra is realized as 3Γ -like symbols which exist whether or not the quotient can be defined as a group. These symbols distribute the value of a reduced matrix element of $SU(2)$ onto the subduced reduced matrix elements of O^* and are termed Partition Coefficients. Since the structure of the excluded symmetry classes is independent of the quantization of O^* , these Partition Coefficients can be used to define the values of the matrix elements of O^* without reference to the form of its basis set. Thus, the choice of physical interpretation of the ligand field is unimportant. The strong field, weak field, Russell-Saunders and $j-j$ coupling models are all unified in terms of the Partition Coefficients and the 3Γ symbols which are appropriate to the quantization.

Key words: Ligand field theory

1. Introduction

In recent analyses of the properties of transition metal complexes, the “intermediate field” model has been introduced to overcome some of the approximations inherent in both the weak and strong field treatments [1–3]. While more powerful than either of these limiting cases, the conventional intermediate field model presents severe computation difficulties and can obscure the interpretation of the chemical parameters. Some attempts have been made to overcome these problems. In particular the concepts of vector coupling have been introduced [1] by extension from either the weak or strong field limits [2, 3] but their use depends on explicit knowledge of the form of the basis functions. In this work, techniques for calculating intermediate field matrix elements will be derived which depend only on the transformation properties and not the algebraic form of the symmetry-adapted eigenvectors of the ligand field.

Traditionally, ligand field models, including the most recent intermediate field formalisms [1–3], have been derived for the analysis of specific metal complexes or specific point

groups. This has emphasized the specific properties of particular symmetries and calculation techniques at the expense of a knowledge of the quantitative relationships between properties of complexes with different symmetries. Such quantitative relationships are inherent in any ligand field model which is derived from considerations of symmetry. These relationships can be specified either in terms of *group characteristics*, that is the full character tables, multiplication of representations and reducibility of representations, or through the behaviour of the vector algebras which are physical realizations of these groups, that is the *algebras of the representations of the groups*.

The algebraic approach has been used in the development of the two presently available intermediate field formalisms [1-3] and in many weak field developments [4]. The group characteristic approach has usually been applied in the strong field limit [5, 6] and for the cubic groups alone in the weak field [7].

Of the two distinct intermediate field models, one is applicable [1] only to O_h and T_d , defined quantized on C_4^z and S_4^z respectively. The other [2, 3] yields parameters which are specific to each realization of each finite group. Neither of these intermediate formalisms nor the traditional weak or strong field models permit the correlation of empirical data between complexes of different symmetries.

In the traditional treatments, this particular shortcoming has been traced to the lack of conceptual clarity and standardization in the definition of the Hamiltonian operators [8-11]. The necessary standardization was achieved by defining the concept of subduction based on the group characteristics. These concepts are independent of the particular ligand field model but do not yield the desired quantitative relationships between the defining concepts and physical parameters of the different models. However, such unifying relationships must exist since we have recently shown that the 3Γ symbols necessary in a strong field model can be derived from the algebra of the weak field basis functions [10, 11]. Conversely the complete set of weak field basis functions can be obtained from the knowledge of a basis set for each J of a single degenerate representation and the 3Γ symbols.

An improved intermediate field formalism is derived in this work through consideration of the characteristics of group lattices [12]. As is shown in this work, the lattice formalism can be further quantified to define the relationships of eigenvalues and eigenvector products between pairs of groups in the lattice. This is done by defining the complementary groups of subduction and the quantitative formalism is derived using Partition Coefficients defined as the 3Γ symbols of the complementary group. These Partition Coefficients which are independent of the axis of quantization describe the distribution of any reduced matrix element into the reduced matrix elements of any subgroup in the lattice.

Partition Coefficients defined in this way can be used to describe the relationships between different realizations of any group and hence between different physical models of a complex. Thus the initial physical interpretation of the operator and hence the basis functions is not crucial because the best features of each realization can be used interchangeably.

Since all subgroups of O_h and T_d can be represented in terms of the tensors of O_h and T_d [4-6] and their associated algebra, the only "intermediate fields" extensively covered will be those represented by the $O_3 \downarrow O_h$ and $O_3 \downarrow T_d$ lattices of groups.

2. Theory

2.1. Group Quotients and Algebras

In conventional ligand field theories the basis functions of a finite point group H can either be defined as perturbed functions of a more symmetric group G , usually $SU(2)$ in a “weak field” model, or within the group H representing the environment, the “strong field” model. Normally, neither classical limit is adequate to fully describe the observables of real complexes. More complete or “intermediate field” solutions are necessary and are classically derived by a perturbation approach from one of the two limits [1-3]. The characteristics of the perturbation differ according to the limit employed and are only understood as algebraic manipulators rather than manifestations of the relationship between the groups G and H .

The nature of the relationship between G and H can be explored by means of the concept of group products and quotients.

Within the strong field model Griffith [6] has shown that if the finite groups H and K are disjoint [12]:

$$H \cup K = E \quad (1)$$

that is H and K have no elements in common except the identity (E); their direct product is another group G :

$$G = H \boxtimes K \quad (2)$$

If the algebras of H and K and the coupling or 3Γ coefficients are known for H and K then the algebra \mathcal{G} , having the representations of G as its elements and the 3Γ symbols of the point group G can be derived from:

$$\mathcal{G} = \mathcal{H} \times \mathcal{K} \quad (3)$$

$$\begin{pmatrix} J_1 & J_2 & J_3 \\ j_1 & j_2 & j_3 \end{pmatrix}_G = \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_H \times \begin{pmatrix} \Delta_1 & \Delta_2 & \Delta_3 \\ \delta_1 & \delta_2 & \delta_3 \end{pmatrix}_K \quad (4)$$

where $\Gamma_i\gamma_i$ or $\Delta_i\delta_i$, $i = 1, 3$, are suitably chosen tensor components of H and K .

Indeed this method for obtaining an algebra or 3Γ ($3-f$) symbols for new groups from disjoint, that is commuting, subgroups is valid for compact and continuous groups [13]. Analogously, algebras and group properties can be defined for non-commuting subgroups by formulation of the semi-direct products. This use of direct and semi-direct products to define the characteristics of the parent group G is usually referred to as the Method of Induction [14, 15].

This method is of limited usefulness since to define G presumes knowledge of K . In the present application of lattices built from physically significant chains of groups it is very difficult to define the complementary group K which may in any case not be unique.

The desired relationship between G and H can instead be derived by defining their quotient [16]:

$$G/H = K \quad (5)$$

H an invariant (normal, central) subgroup of G .

It is easily shown that if H is an invariant subgroup of G the quotient group G/H must be disjoint with respect to H . Hence (5) is an exact inverse of (2). The quotient algebra (“ \mathcal{G} ” algebra in [17]) and the 3Γ coefficients of the quotient group K can be defined [17]:

$$\mathcal{G} | \mathcal{H} = \mathcal{K} \quad (6)$$

and

$$\begin{pmatrix} J_1 & J_2 & J_3 \\ j_1 & j_2 & j_3 \end{pmatrix} \left| \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix} \right. = \begin{pmatrix} \Delta_1 & \Delta_2 & \Delta_3 \\ \delta_1 & \delta_2 & \delta_3 \end{pmatrix} \quad (7)$$

The algebra \mathcal{K} will be a representation algebra of a group if and only if H , the group represented by the algebra \mathcal{H} , is a normal subgroup of G , the group represented by the algebra \mathcal{G} . As pointed out by Coleman [15] however, a quotient algebra $\mathcal{G} | \mathcal{H}$ is always definable irregardless of the existence of K . Thus, while the existence of a simply reducible group G [17] is sufficient to guarantee the existence of the 3Γ symbols it is not, however, a necessary or a minimum [1, 11] condition especially if group lattices are involved. Thus in Eq. (7) the $\begin{pmatrix} \Delta_1 & \Delta_2 & \Delta_3 \\ \delta_1 & \delta_2 & \delta_3 \end{pmatrix}$ symbols for the algebra \mathcal{K} can exist even if the quotient G/H is not a group.

The quotient of interest is $SU(2)/O_h^*$ where $SU(2)$ is the group supporting all the integer and half-integer representations of spin plus orbit angular momentum and O_h^* is the double group for an octahedron including spin coordinates. Since all the coupling coefficients and algebra of O_h^* can be easily derived from O^* [6, 11] the system studied is $SU(2)/O^*$. The $O^* \leftrightarrow T_d^*$ isomorphism is used to obtain the $SU(2)/T_d^*$ algebra and coefficients in Appendix B.

2.2. $SU(2)/O^*$; Quotient Algebra and Coefficients

The properties of a group G reduced with respect to a proper subgroup H , not necessarily a normal subgroup, have been explored by Racah [18] and recently applied to the intermediate [2], strong and weak field formalisms of ligand fields [11]. The central theorem is:

“A realization of a group G always exists such that its eigenvectors are also eigenvectors of H , a proper subgroup of G . This realization of G is then reduced with respect to H .”

When the algebra \mathcal{G} representing G is reduced with respect to H , the elements defining the vector algebra \mathcal{G} , that is the eigenvectors of \mathcal{G} , also form a basis for the vector algebra \mathcal{G} , that is, they are eigenvectors of \mathcal{H} . However, they are not an independent set of eigenvectors for \mathcal{H} , that is, more vectors for \mathcal{H} are defined than are needed.

Several algebrae of $SU(2)$ reduced with respect to realizations of O with different quantization axes have been published [5, 11]. Further the algebra of intermediate fields devel-

oped by Kibler [1] and König [2, 3] is essentially the algebra of an $SU(2)$ or $O(3)$ group reduced with respect to a particular realization of a finite group [8]. However, Eqs. (3, 4, 6, 7) indicate that a quotient algebra approach can profitably be used to describe these intermediate fields.

It will be shown that a unique quotient algebra can be constructed which is independent of the realization of G and H . This algebra represents the connection between the minimum basis set of eigenvectors for \mathcal{H} and the minimum basis set of eigenvectors for \mathcal{G} . Thus, this particular algebra \mathcal{K} quantitatively defines the invariants of the reduction of G onto H which remains implicit in the earlier treatments [1-3].

The quotient algebra is defined rather than the quotient group since a finite group such as O^* is not an invariant subgroup of a compact and continuous, and therefore infinite, group such as $SU(2)$. The complementary group K does not therefore exist in this case. However, several entities, such as coupling coefficients can be defined in the quotient algebra which strongly suggest group properties.

The following derivation is thus algebraic but several properties will be discussed which are suggested by group theoretical considerations.

A change in basis function for an algebra will also change the coupling coefficients for the algebra [6, 17]:

$$\begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1 \gamma_1^* & \Gamma_2 \gamma_2 & \Gamma_3 \gamma_3 \end{pmatrix} = \sum_{M_1 M_2 M_3} \langle J_1 \Gamma_1 \gamma_1 | J_1 M_1 \rangle \langle J_2 \Gamma_2 \gamma_2 | J_2 M_2 \rangle \cdot \langle J_3 \Gamma_3 \gamma_3 | J_3 M_3 \rangle \begin{pmatrix} J_1 & J_2 & J_3 \\ M_1^* & M_2 & M_3 \end{pmatrix} \tag{8}$$

where $\langle J_i \Gamma_i \gamma_i | J_i M_i \rangle$ are the subduction [8-11] coefficients for the group H using the notation due to König [2].

In Eq. (8) the $\begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1^* \gamma_1 & \Gamma_2 \gamma_2 & \Gamma_3 \gamma_3 \end{pmatrix}$ are the 3- j symbols for an $SU(2)$ algebra reduced with

respect to the group H containing representation $\Gamma_i \gamma_i$. Their definition is identical to the F [1, 14] symbols of Kibler. Note that *since they are properties of an $SU(2)$ algebra they must exist regardless of H being a Simply Reducible group*, thus removing some difficulties from their previous interpretation [1]. If proper care is taken in defining the $\Gamma_i \gamma_i$, they can be simply related to the intermediate field coupling coefficient [2, 3].

$$\begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1 \gamma_1 & \Gamma_2 \gamma_2 & \Gamma_3 \gamma_3^* \end{pmatrix} = (-1)^{J_1 - J_2 + \gamma_3^*} [2J_3 + 1]^{-1/2} \langle J_1 \Gamma_1 \gamma_1; J_2 \Gamma_2 \gamma_2 | J_3 \Gamma_3 \gamma_3 \rangle \tag{9}$$

Eqs. (8) and (9) show that the “intermediate fields” as previously developed [1-3], are simply an algebra of $SU(2)$ which is reduced with respect to a subgroup H . However, according to (3), (4), (6) and (7) a much more direct relationship is possible.

2.3. Derivation of Partition Coefficients

According to the Wigner-Eckart theorem and using the notation of Donini *et al.* [19] modified by Eq. (8):

$$\langle l^n J_1 \Gamma_1 \gamma_1 | \ell \Gamma_H \gamma_H | l^n J_2 \Gamma_2 \gamma_2 \rangle = (-1)^{J_1 + \gamma_1^*} \begin{pmatrix} J_1 & \ell & J_2 \\ \Gamma_1 \gamma_1^* & \Gamma_H \gamma_H & \Gamma_2 \gamma_2 \end{pmatrix} \langle l^n J_1 || \ell || l^n J_2 \rangle \quad (10)$$

and further in a strong field sense

$$\langle l^n J_1 \Gamma_1 \gamma_1 | \ell \Gamma_H \gamma_H | l^n J_2 \Gamma_2 \gamma_2 \rangle = (-1)^{J(\Gamma_1) + \gamma_1^*} \begin{pmatrix} \Gamma_1 & \Gamma_H & \Gamma_2 \\ \gamma_1^* & \gamma_H & \gamma_2 \end{pmatrix} \langle l^n J_1 \Gamma_1 || \ell \Gamma_H || l^n J_2 \Gamma_2 \rangle \quad (11)$$

Without loss of generality

$$\begin{aligned} & (-1)^{J_1 + \gamma_1^*} \begin{pmatrix} J_1 & \ell & J_2 \\ \Gamma_1 \gamma_1^* & \Gamma_H \gamma_H & \Gamma_2 \gamma_2 \end{pmatrix} \langle l^n J_1 || \ell || l^n J_2 \rangle \\ &= (-1)^{J(\Gamma_1) + \gamma_1^*} \begin{pmatrix} \Gamma_1 & \Gamma_H & \Gamma_2 \\ \gamma_1^* & \gamma_H & \gamma_2 \end{pmatrix} \langle l^n J_1 \Gamma_1 || \ell \Gamma_H || l^n J_2 \Gamma_2 \rangle \end{aligned} \quad (12)$$

and by application of Eq. (7):

$$\frac{(-1)^{J_1 + \gamma_1^*} \begin{pmatrix} J_1 & \ell & J_2 \\ \Gamma_1 \gamma_1^* & \Gamma_H \gamma_H & \Gamma_2 \gamma_2 \end{pmatrix} \langle l^n J_1 \Gamma_1 || \ell \Gamma_H || l^n J_2 \Gamma_2 \rangle}{(-1)^{J(\Gamma_1) + \gamma_1^*} \begin{pmatrix} \Gamma_1 & \Gamma_H & \Gamma_2 \\ \gamma_1^* & \gamma_H & \gamma_2 \end{pmatrix} \langle l^n J_1 || \ell || l^n J_2 \rangle} = N \quad (13)$$

Because of the definition of reduced matrix elements, the ratio on the R.H.S. of (13) is a number dependent on J_i and Γ_i but independent of γ_i . Defining this number as N , the Eq. (13) can be written:

$$(-1)^{J_1 + \gamma_1^*} \begin{pmatrix} J_1 & \ell & J_2 \\ \Gamma_1 \gamma_1^* & \Gamma_H \gamma_H & \Gamma_2 \gamma_2 \end{pmatrix} = N (-1)^{J(\Gamma_1) + \gamma_1^*} \begin{pmatrix} \Gamma_1 & \Gamma_H & \Gamma_2 \\ \gamma_1^* & \gamma_H & \gamma_2 \end{pmatrix} \quad (14)$$

Squaring both sides and using the appropriate orthonormalization rules (see Appendix A) for real 3 Γ symbols yields:

$$\sum_{\gamma_1 \gamma_H} \begin{pmatrix} J_1 & \ell & J_2 \\ \Gamma_1 \gamma_1^* & \Gamma_H \gamma_H & \Gamma_2 \gamma_2 \end{pmatrix}^2 = N^2 \left(\frac{1}{\lambda[\Gamma_2]} \right) \quad (15)$$

where $\lambda[\Gamma_2]$ is the degeneracy of Γ_2 .

Eqs. (14) and (15) thus identify N up to a phase sign with the N defined as a previously derived normalization coefficient [11], the \bar{V} coefficients of Au-Chin *et al.* [20, 1b] and as isoscalar factors [21].

Because of their independence of γ_i the entities represented by N are called ‘‘Partition Coefficients’’ as discussed in Appendix A. They will be shown to have several very useful properties.

The reduced matrix elements appearing on the R.H.S. of (13) are independent of any unitary transformation which represents an operation within the subgroup H . Such a transformation does not change the block structure of the $SU(2)$ matrix reduced with respect to H but can change the individual entries within the block. These matrix elements are the 3Γ symbols. The reduced matrix elements for \mathcal{H} will not be changed by any unitary transformation which leaves $SU(2)$ reduced with respect to H . Only the subduction coefficients and hence the 3Γ symbols can change.

The relation between different realizations for any group can be expressed as a unitary transformation employing appropriately chosen rotations [6, 22]. Therefore, the value of N is independent of arbitrary choices such as reference axes for the coordinate systems of H and the reference operator of ‘‘quantization’’ of \mathcal{H} [8, 11, 19].

The description of the properties of subgroups of O_h^* and T_d^* in different physically significant chains requires different realizations of O_h^* or T_d^* from $SU(2)$. The proven invariance of the Partition Coefficients allows a unique set to be defined for all quantizations of O_h^* and T_d^* .

A derivation of the normalization and permutation properties of these Partition Coefficients is presented in Appendix A. Since these coefficients are only dependent on J_i , Γ_i and since their properties strongly resemble the $3-j$ or 3Γ symbols they will henceforth be denoted by

$$\begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1 & \Gamma_2 & \Gamma_3 \end{pmatrix}.$$

Following from the Wigner-Eckart theorem or seen as a consequence of Racah’s Lemma [23], Eq. (8) may now be rewritten as:

$$\begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1 \gamma_1^* & \Gamma_2 \gamma_2 & \Gamma_3 \gamma_3 \end{pmatrix} = \begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1 & \Gamma_2 & \Gamma_3 \end{pmatrix} \cdot \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1^* & \gamma_2 & \gamma_3 \end{pmatrix} \quad (16)$$

in terms of Partition Coefficients and 3Γ symbols. Similarly (13) can be rewritten as:

$$\begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1 \gamma_1^* & \Gamma_2 \gamma_2 & \Gamma_3 \gamma_3 \end{pmatrix} \Big/ \begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1 & \Gamma_2 & \Gamma_3 \end{pmatrix} = \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1^* & \gamma_2 & \gamma_3 \end{pmatrix} \quad (17)$$

and the strict relationship between the Partition Coefficient and the $3\Gamma(3-j)$ symbols of a quotient group is now apparent by simply comparing (4) and (7) with (16) and (17).

2.4. Calculation of Partition Coefficients

The expansion of the L.H.S. of (10) in terms of 3- j symbols is used to calculate the Partition Coefficients, i.e.:

$$\begin{aligned} \left(\begin{array}{ccc} J_1 & J_2 & J_3 \\ \Gamma_1 & \Gamma_2 & \Gamma_3 \end{array} \right) &= \frac{(-1)^{J_1 + \gamma_1^*} \left(\begin{array}{ccc} J_1 & J_2 & J_3 \\ \Gamma_1 \gamma_1^* & \Gamma_2 \gamma_2 & \Gamma_3 \gamma_3 \end{array} \right)}{(-1)^{J(\Gamma_1) + \gamma_1^*} \left(\begin{array}{ccc} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1^* & \gamma_2 & \gamma_3 \end{array} \right)} = \\ &= \frac{\sum_{M_1, M_2, M_3} (-1)^{J_1 - M_1} \langle J_1 \Gamma_1 \gamma_1 | J_1 M_1 \rangle^* \langle J_2 \Gamma_2 \gamma_2 | J_2 M_2 \rangle \langle J_3 \Gamma_3 \gamma_3 | J_3 M_3 \rangle \left(\begin{array}{ccc} J_1 & J_2 & J_3 \\ M_1^* & M_2 & M_3 \end{array} \right)}{(-1)^{J(\Gamma_1) + \gamma_1^*} \left(\begin{array}{ccc} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1^* & \gamma_2 & \gamma_3 \end{array} \right)} \end{aligned} \quad (18)$$

This definition differs from the F symbols of Kibler [1b] by the phase factors depending on $(J_1 - M_1)$ and $(\Gamma_1 + \gamma_1^*)$. In the V coefficients [20], the phases of T_1 and T_2 are identical rather than depending on $J(\Gamma_i)$. In both cases these signs appear in the reduced matrix element of the strong field. Since all phase signs are explicitly included in the present definition (18), the relationship between the finite group and infinite group reduced matrix element is defined as:

$$\langle J_1 \| \ell \| J_2 \rangle \left(\begin{array}{ccc} J_1 & \ell & J_2 \\ \Gamma_1 & \Gamma_H & \Gamma_2 \end{array} \right) = \langle J_1 \Gamma_1 \| \ell \Gamma_H \| J_2 \Gamma_2 \rangle \quad (19)$$

with no phase factors.

Substituting for (19) in (11), the basic equation for application of the 3Γ symbols and Partition Coefficients is obtained:

$$\begin{aligned} \langle I^n J_1 \Gamma_1 \gamma_1 | \ell \Gamma_H \gamma_H | I^n J_2 \Gamma_2 \gamma_2 \rangle &= (-1)^{J(\Gamma_1) + \gamma_1^*} \left(\begin{array}{ccc} \Gamma_1 & \Gamma_H & \Gamma_2 \\ \gamma_1^* & \gamma_H & \gamma_2 \end{array} \right) \left(\begin{array}{ccc} J_1 & \ell & J_2 \\ \Gamma_1 & \Gamma_H & \Gamma_2 \end{array} \right) \times \\ &\times \langle I^n J_1 \| \ell \| I^n J_2 \rangle \end{aligned} \quad (20)$$

Since the Partition Coefficients and the Reduced Matrix Elements (R.M.E.) are independent of the realization of H , the only difference between different realizations and quantizations is held in the 3Γ symbols. Tables of 3Γ or coupling coefficients defined with respect to the most useful realization and quantization are available [5, 10, 11, 24]. However, great care must be taken since only two [10, 11] employ a sign convention compatible with the present derivation of Partition Coefficients.

One of the major drawbacks encountered in the strong field formalism is the difficulty in calculating the Reduced Matrix Element. Eqs. (19) and (20) relieve this difficulty by

solving the finite group R.M.E. in terms of the R.M.E. occurring in $SU(2)$ or (R_3) and permit the use of the excellent tabulations of Nielson and Köster [26].

Partition Coefficients are intended for use in equations such as (19) and (20). Since several restrictions can be imposed upon the nature of the crystal field Hamiltonian $\ell\Gamma_M\gamma_M$, only Partition Coefficients containing allowed $\ell\Gamma_M\gamma_M$ have been calculated. The restrictions imposed on $\ell\Gamma_M\gamma_M$ in the case of $d \rightarrow d$ or $f \rightarrow f$ transition are:

1. ℓ even and ≤ 6 [8, 19, 24],
2. Γ_H either A_1, E or T_2 [8-11].

E.P.R. results and magnetic susceptibilities can also be calculated by these methods [1-3]. To allow for such calculations, the Partition Coefficients for $\ell = 1, \Gamma = T_1$ (the electric or magnetic tensor in O) or $\Gamma = T_2$ (the electric tensor in T_d , see Appendix B), have also been calculated. Similarly the $\ell = 0, \Gamma_H = A_1$ case has been included as it represents a convenient bench-mark for accuracy as well as being of use in spin-orbit coupling calculations. Notwithstanding Eqs. (19) and (20), Eqs. (8), (16) and (17) imply a much greater applicability of Partition Coefficients. Care, however, must be taken with regard to phase factors when applications other than those suggested by (18) and (19) are envisaged.

3. Applications of Partition Coefficients

3.1. Group Lattices [12]

The quantum numbers chosen to represent a particular wave function and indeed the form of the basis set used to define the properties of a system depend on various assumptions about the relative importance of various effects, such as inter-electronic repulsion (I.E.R.), spin-orbit coupling ($\lambda_{L.S.}$) and the crystal field ($V_{C.F.}$). Each possible arrangement corresponds to a particular [12] realization of the groups in the chain from $(O(3))^N$, the group of N electrons in $O(3)$, to G , the group describing the physical environment. A diagram showing several such possible choices is called a lattice diagram [12]. These choices do not affect the final eigenvalue if all possible interactions between different elements of the basis set are taken into account. The different choices, however, do affect the form of the basis set and also the way various interactions are calculated with respect to the chosen basis set.

The formalism of intermediate fields and their attendant Partition Coefficients offer a single method of calculation for all elements in the lattice. Consider, for example, the case for a d^N ion in a D_{3d} field; the Hamiltonian is:

$$H = H_0 \times I + \left(\sum_{i < j} \frac{e^2}{r_{ij}} \right) \times I + \sum_i L \cdot S_i + H(O_h) \times I + H(D_{3d}) \times I \quad (21)$$

where all operators are written as products of orbital and spin terms. The individual parts of the Hamiltonian can be identified as:

I = Identity for the Simplectic Unitary Group, $SU(2)$ (Spin Group).

H_0 = Hydrogenic Hamiltonian.

$\sum_{i < j} \frac{e^2}{r_{ij}}$ = Inter-electronic repulsion

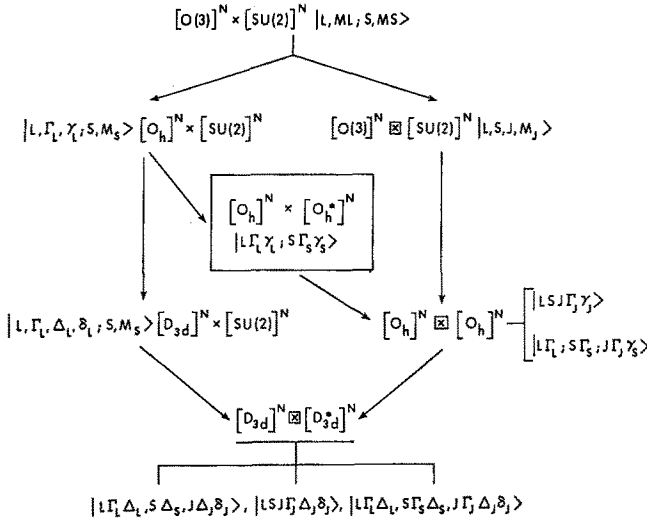


Fig. 1. The lattice of groups and supporting wave functions for the $SU(2) \downarrow D_{3d}^*$ chains of groups. \times = semidirect product of groups (ordered pairs), \boxtimes = direct product of groups, $[G]^N = N$ th direct product of G with itself which is a group that represents N identical particles in an environment of symmetry G

$$\sum_i L \cdot S_i = \text{Spin-orbit coupling.}$$

$H(O_h)$ = Hamiltonian for an octahedral O_h field.

$H(D_{3d})$ = Hamiltonian for a trigonal D_{3d} field.

The lattice thus generated is displayed in Fig. 1.

Fig. 2 is a possible correlation diagram for $N = 1$. This correlation diagram is obtained by simply inverting relative order of application of the crystal field and spin-orbit coupling operators and therefore is a Russell-Saunders to $j-j$ coupling correlation diagram. Other such diagrams can be obtained by inverting the relative order of inter-electronic repulsion and the crystal field in a many-electron atom giving rise to a strong field (crystal field strongest) to weak field (I.E.R. strongest) correlation diagram. The final solution will always be contained in the column headed $\Gamma(D_{3d}^*)$ and the eigenvalues obtained are independent of the route used in obtaining them, if a complete calculation is undertaken. Thus the choice of route is a matter of convenience.

3.2. Alternate Formulae for Application

The number of practical realizations of the basis functions of finite groups is quite limited. One choice is through the left part of the lattice in Fig. 2. This route is useful if spin-orbit coupling is not important and no E.P.R. or magnetic susceptibility data are to be fitted. In this approach the basis set at the $[O(3)]^N \times [SU(2)]^N$ level is of form $|l^n L, S, M_L, M_S\rangle$. Since all subgroups of O_h are solved in terms of O_h tensors the proper form for the basis set of $[O_h]^N \times [SU(2)]^N$ is:

$$|l^n, L, S, \Gamma_1 \gamma_1, M_S\rangle$$

where $\Gamma_1 \gamma_1$ are a representation Γ_i and component γ_i derived from L in the group O_h .

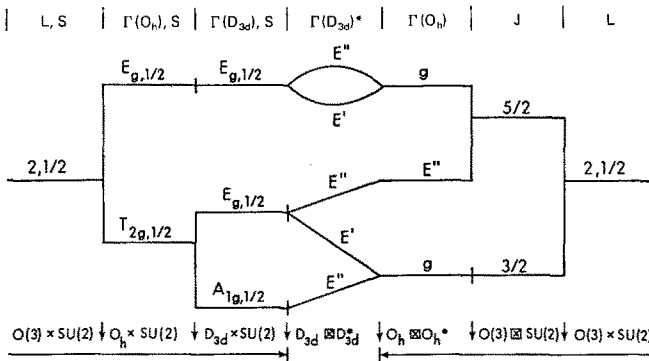


Fig. 2. Correlation diagram of the Russell-Saunders and *j-j* formalisms in a $d^1 D_{3d}^*$ system

The matrix elements due to the crystal field in the case of a D_{3d} symmetry are of form:

$$\begin{aligned}
 & \langle l^n, L, S, \Gamma_l \gamma_l, M_S | DQ4A_1 0 + DS2T_2 0 + DT4T_2 0 | l^n L', S', \Gamma'_l \gamma'_l, M'_S \rangle \\
 & = \delta_{SS'} \cdot \delta_{M_S M'_S} \left[\left\{ (-1)^{J(\Gamma_l) + \gamma_l^*} \begin{pmatrix} \Gamma_l & A_1 & \Gamma'_l \\ \gamma_l^* & 0 & \gamma'_l \end{pmatrix} \begin{pmatrix} L & 4 & L' \\ \Gamma_l & A_1 & \Gamma'_l \end{pmatrix} DQ \right. \right. \\
 & \quad + (-1)^{J(\Gamma_l) + \delta l^*} \begin{pmatrix} \Gamma_l & T_2 & \Gamma'_l \\ \gamma_l^* & 0 & \gamma'_l \end{pmatrix} \begin{pmatrix} L & 4 & L' \\ \Gamma_l & T_2 & \Gamma'_l \end{pmatrix} DT \left. \langle l^n L || 4 || l^n L' \rangle \right. \right. \\
 & \quad \left. \left. + (-1)^{J(\Gamma_l) + \gamma_l^*} \begin{pmatrix} \Gamma_l & T_2 & \Gamma'_l \\ \gamma_l^* & 0 & \gamma'_l \end{pmatrix} \begin{pmatrix} L & 2 & L' \\ \Gamma_l & T_2 & \Gamma'_l \end{pmatrix} DS \langle l^n L || 2 || l^n L' \rangle \right\} \quad (22)
 \end{aligned}$$

where $4A_1 0$ means the 0 component of A_1 from the $L = 4$ spherical harmonics and similarly for $2T_2 0$ and $4T_2 0$; DQ, DS, DT are the empirical parameters which are varied

to fit the experimental data; and $\begin{pmatrix} \Gamma_l & A_1 & \Gamma'_l \\ \gamma_l^* & 0 & \gamma'_l \end{pmatrix}$ are the 3Γ symbols defined with respect to

the appropriate quantization system (C_3^z in this case), $\langle l^n L || \ell || l^n L' \rangle \ell = 2, 4$ are the reduced matrix elements, which are available in tabular form [26].

Eq. (21) can be solved without knowledge of the particular linear combinations of H and M_L giving rise to the $|\Gamma_l \gamma_l\rangle$ functions. All of the information necessary is contained in the 3Γ and Partition Coefficients.

If spin-orbit coupling is to be calculated and E.P.R. and magnetic susceptibility data are to be fitted it is much more convenient to operate on the group $[12] [O(3)]^N \boxtimes [SU(2)]^N$ in which \boxtimes implies an inner subdirect product, represented by a basis set of form:

$$|l^n, L, S, J, M\rangle \quad (23)$$

which when adapted to the $[O_h]^N \boxtimes [O_h^*]^N$ group supports a basis set of type:

$$|l^n L, S, J, \Gamma_l \gamma_l\rangle \quad (24)$$

This alternative is represented by the L.H.S. of Figs. 1 and 2.

Since the spin-orbit coupling matrix elements are independent of M and since the $\Gamma_j \gamma_j$ of Eq. (24) are simply orthonormal linear combinations of M in Eq. (23), the matrix elements of a basis of form (24) are identical to those of form (23) and are therefore well known [23, 27, 28]. The formula will be reported for completeness but it does not involve partition coefficients:

$$\begin{aligned} & \langle l^n, \alpha, L, S, J, M | \xi L \cdot S | l^n, \alpha', L', S', J', M' \rangle \\ &= \langle l^n, \alpha, L, S, J, \Gamma_J \gamma_J | \lambda L \cdot S | l^n, \alpha', L', S', J', \Gamma'_J \gamma'_J \rangle \\ &= \xi \delta_{J, J'} \cdot \delta_{M, M'} \cdot \delta_{\Gamma_J \gamma_J, \Gamma'_J \gamma'_J} (-1)^{J-L-S'} [l(l+1)(2l+1)]^{1/2} \begin{pmatrix} S & L & J \\ L' & S' & 1 \end{pmatrix} \\ & \langle l^n, \alpha, L, S || V^{11} || l^n, \alpha, L, S \rangle \end{aligned} \quad (25)$$

where the $\langle l^n L S || V^{11} || l^n L' S' \rangle$ are the reduced matrix elements [26].

Since ligand field Hamiltonians only act on L and M_L , some difficulty arises in calculating this effect on the JM basis. The problem has, however, been solved [28, 29] and application of the same techniques on the present case yields:

$$\begin{aligned} & \langle l^n, \alpha, L, S, J, \Gamma_J \gamma_J | \kappa; \Gamma_H \gamma_H | l^n, \alpha', L', S', J', \Gamma'_J \gamma'_J \rangle \\ &= (-1)^{J(\Gamma_J) + \gamma_J^* + S + \kappa - L - 2L' - J - J'} [(2J+1)(2J'+1)]^{1/2} \begin{pmatrix} \Gamma_J & \Gamma_H & \Gamma'_J \\ \gamma_J^* & \gamma_H & \gamma'_J \end{pmatrix} \\ & \cdot \begin{pmatrix} J & \kappa & J' \\ \Gamma_J & \Gamma_H & \Gamma'_J \end{pmatrix} \begin{pmatrix} L & J & S \\ J' & L' & \kappa \end{pmatrix} \langle l^n, \alpha, L, S || C^\kappa || l^n, \alpha, L', S \rangle \end{aligned} \quad (26)$$

where the $\begin{pmatrix} L & J & S \\ J' & L' & \kappa \end{pmatrix}$ are the 6- j symbols [30].

If the interactions of the basis set under either the magnetic (T_1 in O_h) or electronic (T_1 in O_h) dipole operators are needed, the development by Gerloch [28] can be modified appropriately.

Using T_1 to signify either T_{1g} or T_{1u} as necessary:

$$\begin{aligned} & \langle l^n, \alpha, L, S, J, \Gamma_J \gamma_J | 1T_1 0 | l^n, \alpha', L', S', J', \Gamma'_J \gamma'_J \rangle \\ &= (-1)^{J(\Gamma_J) + \gamma_J^*} \begin{pmatrix} \Gamma_J & T_1 & \Gamma'_J \\ \gamma_J & 0 & \gamma'_J \end{pmatrix} [x] \end{aligned} \quad (27)$$

$$P_z, \hat{\mu}_z \equiv C_1^0 \equiv (T_1 0) \quad (28)$$

and

$$\begin{aligned} & \left\langle l^n, \alpha, L, S, J, \Gamma_J \gamma_J \left| 1 \left(\frac{1}{\sqrt{2}} (-T_1 1) + (T_1 - 1) \right) \right| l^n, \alpha', L', S', J', \Gamma'_J \gamma'_J \right\rangle \\ &= \frac{(-1)^{J(\Gamma_J) + \gamma_J^*}}{\sqrt{2}} \left[\begin{pmatrix} \Gamma_J & T_1 & \Gamma'_J \\ \gamma_J^* & -1 & \gamma'_J \end{pmatrix} - \begin{pmatrix} \Gamma_J & T_1 & \Gamma'_J \\ \gamma_J^* & 1 & \gamma'_J \end{pmatrix} \right] [x] \end{aligned} \quad (29)$$

where in the case of three and four-fold quantized systems:

$$\frac{1}{\sqrt{2}}(-(T_1 1) + (T_1 - 1)) = \frac{1}{\sqrt{2}}(-C_1^1 + C_1^{-1}) = \hat{\mu}_x, P_x \tag{30}$$

for two-fold systems:

$$(T_1 1-) = \frac{1}{\sqrt{2}}(C_1^1 - C_1^{-1}) = -\hat{\mu}_x, -P_x \tag{31}$$

and hence appropriate changes are made in (28).

In (27), (29) and (30) μ stands for the magnetic dipole operator while P_x is the electric dipole operator.

In the case of magnetic susceptibilities, the operator is μ , or $(L + 2S)$ in the more usual Zeeman operator form. Hence the factor $[\chi]$ of Eqs. (27) and (29) becomes:

$$[\chi] = \begin{pmatrix} J & 1 & J' \\ \Gamma_J & T_1 & \Gamma_J' \end{pmatrix} [(2J + 1)(2J' + 1)]^{1/2} \left[[L(L + 1)(2L + 1)]^{1/2} \cdot \begin{pmatrix} J & 1 & J' \\ L & S & L' \end{pmatrix} + 2[S(S + 1)(2S + 1)]^{1/2} \begin{pmatrix} J & 1 & J' \\ S & L & S \end{pmatrix} \right] \tag{32}$$

the preceding is a reduced matrix element in two parts; one pertaining to L operating on the orbital part of the wave function and the other representing $2S$ operating on the spin part of the wave function.

A different definition of $[\chi]$ is necessary for the calculation of E.P.R. results and can be easily derived [1].

A third method of calculation does exist and is represented in Fig. 1 by the diagonal line connecting $[12] [O_h J^N] \times [SU(2)]^N$ to $[O_h]^N \times [O_h^*]^N$. It requires a basis set of the form:

$$|l^n, \alpha, L, \Gamma_L, S, \Gamma_S, J, \Gamma_J \gamma_J\rangle \tag{33}$$

and has been employed by König *et al.* [2, 3].

The application of Partition Coefficients to these bases illustrates a different use from the one suggested by their derivation. The Partition Coefficients are used in a way strongly reminiscent of coupling coefficients and thus illustrate even more vividly the connections between Partition Coefficients and 3- j coupling symbols of a quotient group.

The ligand field operator (21) acting only on the $|LM_L\rangle$ functions (33) can be written as $H_L \times I$ when I is the identity of the group $SU(2)$. In terms of tensors coupled to a $|J\Gamma_J\gamma_J\rangle$ the operator is;

$$|L_H \Gamma_{HL}, S_H \Gamma_{HS}, J_H \Gamma_{HJ} \gamma_{HJ}| = |\ell A_1, 0A_1, \ell JA, 0|$$

$$\begin{aligned} \ell A_1 &= A_1 && \text{for } L = \ell, \text{ operating on } LM_L \text{ only} \\ 0A_1 &= A_1 && \text{for } L = 0, \text{ operating on } SM_S \text{ only (Identity of } SU(3)). \\ \ell JA_1 &= A_1 && \text{for } J = \ell, \text{ operating on } J \end{aligned} \tag{34}$$

and hence a matrix element has the form:

$$\begin{aligned} & \langle l^n, \alpha, L\Gamma_L, S\Gamma_S, J\Gamma_J \gamma_J | \ell A_1, 0A_1, kJA_1 0 | l^n, \alpha', L'\Gamma'_L, S'\Gamma'_S, J\Gamma'_J \gamma'_J \rangle \\ & = (-1)^{J(\Gamma_J) + \gamma_J} \begin{pmatrix} \ell & 0 & k \\ A_1 & A_1 & A_1 \end{pmatrix} \frac{(2\ell+1)}{\lambda[A_1]} \begin{pmatrix} L & S & J \\ \Gamma_L & \Gamma_S & \Gamma_J \end{pmatrix} \frac{(2J+1)}{\lambda[\Gamma_J]} \begin{pmatrix} L' & S' & J' \\ \Gamma'_L & \Gamma'_S & \Gamma'_J \end{pmatrix} \frac{(2J'+1)}{\lambda[\Gamma'_J]} \\ & \cdot \langle l^n, \alpha, L, S, J | \ell, 0, \ell | l^n, \alpha', L', S', J' \rangle \end{aligned} \quad (35)$$

But from Eq. (A1.10):

$$\begin{pmatrix} \ell & 0 & \ell \\ A_1 & A_1 & A_1 \end{pmatrix} \frac{(2\ell+1)}{\lambda[A_1]} = 1 \quad (36)$$

Under this condition the R.H.S. of Eq. (35) becomes:

$$\begin{aligned} & = (-1)^{J(\Gamma_J) + \gamma_J} \frac{[(2J+1)(2J'+1)]^{1/2}}{\lambda[\Gamma_J]\lambda[\Gamma'_J]} \begin{pmatrix} L & S & J \\ \Gamma_L & \Gamma_S & \Gamma_J \end{pmatrix} \begin{pmatrix} L' & S' & J' \\ \Gamma'_L & \Gamma'_S & \Gamma'_J \end{pmatrix} \\ & \cdot \begin{pmatrix} \Gamma_J & \ell & \Gamma'_J \\ \gamma_J & 0 & \gamma'_J \end{pmatrix} \langle l^n, \alpha, L, S, J | \ell, 0, \ell | l^n, \alpha', L', S', J' \rangle \end{aligned} \quad (37)$$

and the reduced matrix element $\langle l^n, \alpha, L, S, J | \ell, 0, \ell | l^n, \alpha', L', S', J' \rangle$ can be solved using Eq. (26).

4. Conclusion

Application of the appropriate equation makes it possible to solve all the different branches of a lattice diagram [12] (Fig. 1) in terms of a single formalism involving Partition Coefficients, 3Γ symbols [10, 11], $6-j$ symbols [30] and reduced matrix elements [26].

Within the formalism developed in this paper it is not necessary to know the actual form of the wave function. Lengthy tabulations of subduction coefficients become obsolete [5, 10, 11, 19, 24] and are replaced by the knowledge of the appropriate 3Γ symbols [10, 11] or equivalent entities [5, 6, 24] and Partition Coefficients. Further correlation tables [12] such as in Fig. 2 can now be obtained quantitatively. Different branches of these correlation tables correspond to a different quantization of the eigenfunctions yielding the desired eigenvalues. Thus all the various aspects of classical crystal fields such as strong and weak field approximations and the Russell-Saunders and $j-j$ coupling models have been united in terms of a covering formalism relying on the existence of a quotient algebra K .

Eqs. (25–31) in particular have been used to calculate the characteristics of spectra of tetrahedral Co [31] and rhombohedral Eu^{3+} [32] complexes with a considerable reduction of computer time and space [19].

All the calculations necessary to calculate Partition Coefficients and interaction matrices have been accomplished on a 32K, 16 bit word mini-computer. Even greater savings of space and time can be achieved when magnetic properties are to be investigated [33].

The formalism and properties of Partition Coefficients when coupled to the concepts of Normalized Spherical Harmonic (N.S.H.) Hamiltonians [8, 9], physically significant chains of groups [8-10] and sequence adapted wave functions [8-11, 34] concludes exploration of group theoretical techniques aimed at obtaining linearly independent, mutually orthogonal [35] Hamiltonians which can be used to obtain useful chemical information [4, 5, 19] from complexes of symmetry lower than O_h and T_d . The outstanding problem is the understanding of the meaning of the empirical parameters DQ , DS , B , C and λ . Quotient groups techniques can be used in this latter context [13, 37-39] and are being actively investigated with the intent to obtain an *a priori* estimate for the various empirical parameters of crystal fields.

Appendix A. Properties of Partition Coefficients

A.1. Orthonormalization Properties

Substituting the Partition Coefficient notation for N in (14) yields;

$$(-1)^{J_1+\gamma_1^*} \begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1 \gamma_1^* & \Gamma_2 \gamma_2 & \Gamma_3 \gamma_3 \end{pmatrix} = (-1)^{J(\Gamma_1)+\gamma_1^*} \begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1 & \Gamma_2 & \Gamma_3 \end{pmatrix} \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1^* & \gamma_2 & \gamma_3 \end{pmatrix} \quad (\text{A1.1})$$

All the entities are real numbers and can therefore be squared to obtain;

$$\begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1 \gamma_1^* & \Gamma_2 \gamma_2 & \Gamma_3 \gamma_3 \end{pmatrix}^2 = \begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1 & \Gamma_2 & \Gamma_3 \end{pmatrix}^2 \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1^* & \gamma_2 & \gamma_3 \end{pmatrix}^2 \quad (\text{A1.2})$$

Written in a more usual form and summed over $\gamma_1 \gamma_2$ (A1.2) yields;

$$\begin{aligned} & \sum_{\gamma_1 \gamma_2} \begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1 \gamma_1^* & \Gamma_2 \gamma_2 & \Gamma_3 \gamma_3 \end{pmatrix} \begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1 \gamma_1^* & \Gamma_2 \gamma_2 & \Gamma_3 \gamma_3 \end{pmatrix} \\ & = \sum_{\gamma_1 \gamma_2} \begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1 & \Gamma_2 & \Gamma_3 \end{pmatrix} \begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1 & \Gamma_2 & \Gamma_3 \end{pmatrix} \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1^* & \gamma_2 & \gamma_3 \end{pmatrix} \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1^* & \gamma_2 & \gamma_3 \end{pmatrix} \end{aligned} \quad (\text{A1.2})$$

However, the Partition Coefficients are independent of γ_1^* , γ_2 , γ_3 and therefore the summation on the R.H.S. of (A1.3) only affects the 3Γ symbols and is in fact the orthonormalization condition for 3Γ symbols. Thus;

$$\sum_{\gamma_1 \gamma_2} \begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1 \gamma_1^* & \Gamma_2 \gamma_2 & \Gamma_3 \gamma_3 \end{pmatrix} \begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1 \gamma_1^* & \Gamma_2 \gamma_2 & \Gamma_3 \gamma_3 \end{pmatrix} = \frac{1}{\lambda[\Gamma_3]} \begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1 & \Gamma_2 & \Gamma_3 \end{pmatrix} \begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1 & \Gamma_2 & \Gamma_3 \end{pmatrix} \quad (\text{A1.4})$$

where $\lambda[\Gamma_3] = \text{degeneracy of } \Gamma_3$. This is Eq. (15) of the main text.

The symbols for the intermediate fields are the $3-j$ symbols of an $SU(2)$ group which is defined to be reduced with respect to its subgroup O [11]. The relationship between these $3-j$ symbols and the standard $3-j$ symbols is a unitary transformation. The subduction coefficients $\langle J_i \Gamma_i \gamma_i | J_i M_i \rangle$ of (8) are the individual matrix elements of the unitary transformation matrix. However, multiplication by a unitary matrix does not effect orthonormaliza-

tion properties of a matrix or its eigenvectors and therefore

$$\sum_{\Gamma_1 \gamma_1, \Gamma_2 \gamma_2} \begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1 \gamma_1^* & \Gamma_2 \gamma_2 & \Gamma_3 \gamma_3 \end{pmatrix}^2 = \sum_{M_1, M_2} \begin{pmatrix} J_1 & J_2 & J_3 \\ M_1^* & M_2 & M_3 \end{pmatrix}^2 = \frac{1}{(2J_3 + 1)} \quad (\text{A1.5})$$

Summation of (A1.4) over $\Gamma_1 \Gamma_2$ yields;

$$\sum_{\Gamma_1 \gamma_1, \Gamma_2 \gamma_2} \begin{pmatrix} J_2 & J_2 & J_3 \\ \Gamma_1 \gamma_1^* & \Gamma_2 \gamma_2 & \Gamma_3 \gamma_3 \end{pmatrix}^2 = \frac{1}{\lambda[\Gamma_3]} \sum_{\Gamma_2, \Gamma_3} \begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1 & \Gamma_2 & \Gamma_3 \end{pmatrix}^2 \quad (\text{A1.6})$$

which when substituted with (A1.5) yields

$$\sum_{\Gamma_1 \Gamma_2} \begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1 & \Gamma_2 & \Gamma_3 \end{pmatrix}^2 = \frac{\lambda[\Gamma_3]}{(2J_3 + 1)} \quad (\text{A1.7})$$

This last equation is an orthonormalization relationship very similar to those for 3- j or 3 Γ symbols. It also suggests that a "coupling coefficient" can be defined for the Partition Coefficient and indeed if (8) is restated in terms of coupling coefficients rather than 3- j symbols then it follows that

$$\begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1 & \Gamma_2 & \Gamma_3 \end{pmatrix} = (-1)^{J_1 - J_2 - J(\Gamma_3)} \left[\frac{\lambda[\Gamma_3]}{(2J_3 + 1)} \right]^{-1/2} \langle J_1 \Gamma_1, J_2 \Gamma_2 | J_3 \Gamma_3 \rangle \quad (\text{A1.8})$$

Another orthonormalization condition is defined for 3- j or 3 Γ symbols. This condition can be extended to the intermediate Field 3- j symbols

$$\sum_{J_3, M_3} (2J_3 + 1) \begin{pmatrix} J_1 & J_2 & J_3 \\ M_1^* & M_2 & M_3 \end{pmatrix}^2 = \sum_{J_3, \Gamma_3 \gamma_3} (2J_3 + 1) \begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1 \gamma_1^* & \Gamma_2 \gamma_2 & \Gamma_3 \gamma_3 \end{pmatrix}^2 = 1 \quad (\text{A1.9})$$

A realization of H such that a specific $\Gamma_1 \gamma_1 \boxtimes \Gamma_1 \gamma_2$ only yields one $\Gamma_3 \gamma_3$ is always possible [40]. In this particular realization the summation of $\Gamma_3 \gamma_3$ in the R.H.S. of (A1.9) is redundant just as the summation over M_3 of the L.H.S. is redundant because of the condition $M_1^* + M_2 = -M_3$. Thus for this particular realization labelled P

$$\sum_{J_3} (2J_3 + 1) \begin{pmatrix} J_1 & J_2 & J_3 \\ M_1^* & M_2 & M_3 \end{pmatrix}^2 = \sum_{J_3} (2J_3 + 1) \begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1 \gamma_1^* & \Gamma_2 \gamma_2 & \Gamma_3 \gamma_3 \end{pmatrix}_P^2 \quad (\text{A1.9B})$$

The Partition Coefficients are independent of the realizations of H and therefore all the properties proved by using this particular realization are of general validity.

Since [1];

$$\sum_{\Gamma_3 \gamma_3} \frac{1}{\lambda[\Gamma_3]} \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1^* & \gamma_2 & \gamma_3 \end{pmatrix}^2 = 1$$

it follows that;

$$\begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1^* & \gamma_2 & \gamma_3 \end{pmatrix}_P^2 = \lambda[\Gamma_3]$$

and therefore in this particular realization, and no other, (A1.2) is;

$$\begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1 & \Gamma_2 & \Gamma_3 \end{pmatrix}^2 = \begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1 \gamma_1^* & \Gamma_2 \gamma_2 & \Gamma_3 \gamma_3 \end{pmatrix}_P^2 \lambda[\Gamma_3]$$

and, by analogy to (A1.9B);

$$\sum_{J_3} (2J_3 + 1) \begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1 & \Gamma_2 & \Gamma_3 \end{pmatrix}^2 = \sum_{J_3} (2J_3 + 1) \begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1 \gamma_1^* & \Gamma_2 \gamma_2 & \Gamma_3 \gamma_3 \end{pmatrix}_P^2 \lambda[\Gamma_3]$$

Transposing the $\lambda[\Gamma_3]$ and applying the particular orthonormalization (A1.9B) yields the desired result:

$$\sum_{J_3} \frac{(2J_3 + 1)}{\lambda[\Gamma_3]} \begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1 & \Gamma_2 & \Gamma_3 \end{pmatrix}^2 = 1 \quad (\text{A1.10})$$

Eqs. (A1.7) (A1.9) (A1.10) have been derived previously with regard to O quantized on the four-fold axis, by different methods [20]. These equations, together with Eq. (A1.8), clearly show the strict parallelism between the Partition Coefficients and the $3-j$ and 3Γ symbols.

A.2. Root Weight

The orthonormalization condition (A1.10) can be used to reveal the strict relationship between the $3-j$ symbol of $SU(2)$ reduced with respect to a particular realization \mathcal{H} of H and the 3Γ symbols of \mathcal{H} . To do so (A1.2) is suitably modified by multiplication of appropriate factors and summation on both the left- and right-hand sides

$$\sum_{J_3} \frac{(2J_3 + 1)}{\lambda[\Gamma_3]} \begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1 \gamma_1^* & \Gamma_2 \gamma_2 & \Gamma_3 \gamma_3 \end{pmatrix} = \sum_{J_3} \frac{(2J_3 + 1)}{\lambda[\Gamma_3]} \begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1 & \Gamma_2 & \Gamma_3 \end{pmatrix}^2 \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1^* & \gamma_2 & \gamma_3 \end{pmatrix}^2$$

since the 3Γ symbols are independent of J_i ;

$$\begin{aligned} \sum_{J_3} (2J_3 + 1) \begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1 \gamma_1^* & \Gamma_2 \gamma_2 & \Gamma_3 \gamma_3 \end{pmatrix}^2 &= \lambda[\Gamma_3] \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1^* & \gamma_2 & \gamma_3 \end{pmatrix}^2 \sum_{J_3} \frac{(2J_3 + 1)}{\lambda[\Gamma_3]} \times \\ &\times \begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1 & \Gamma_2 & \Gamma_3 \end{pmatrix}^2 \end{aligned}$$

Application of (A1.10) then yields;

$$\sum_{J_3} (2J_3 + 1) \begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1 \gamma_1^* & \Gamma_2 \gamma_2 & \Gamma_3 \gamma_3 \end{pmatrix}^2 = \lambda[\Gamma_3] \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1^* & \gamma_2 & \gamma_3 \end{pmatrix}^2 \quad (\text{A1.11})$$

which, by application of the relationships between coupling coefficients on $3-j$ [27] and 3Γ [10, 11] symbols, is reduced to;

$$\sum_{J_3} \langle J_2 \Gamma_1 \gamma_1, J_2 \Gamma_2 \gamma_2 | J_3 \Gamma_3 \gamma_3 \rangle^2 = \langle \Gamma_1 \gamma_1, \Gamma_2 \gamma_2 | \Gamma_3 \gamma_3 \rangle^2 \quad (\text{A1.12})$$

Since the R.H.S. of the last equation is independent of J values it is clearly a property of the algebra of H only and is independent of the coupling in $SU(2)$.

Eqs. (A1.11 and 12) provide a way to derive the absolute magnitude of the 3Γ symbols from the $3-j$ of the reduced $SU(2)$. This technique offers several advantages over an alternate method [10]. Both of these methods have been used recently [11] to derive extensive sets of 3Γ symbols for O_h and T_d realized with respect to several different quantizing conditions.

Eqs. (A1.11 and 12) can be interpreted as a definition of the Root Weight of the coupling $\Gamma_1 \gamma_1 \times \Gamma_2 \gamma_2$ to yield $\Gamma_3 \gamma_3$ in a realization \mathcal{H} of H embedded in a $SU(2)$ space. Even though these equations are independent of the Partition Coefficients, a clear understanding of the properties of the Partition Coefficients is necessary to derive (A1.11, 12).

A.3. Permutation Properties and Existence

The permutation properties are easily derived from (18) and the individual permutation properties of the $3-j$ and 3Γ symbols. Thus using the notation of (7) for the 3Γ symbols;

$$(-1)^{J_1+J(\Gamma_1)} \begin{pmatrix} J_1 & J_2 & J_3 \\ \Gamma_1 & \Gamma_2 & \Gamma_3 \end{pmatrix} = (-1)^{J_1+2J_2+J_3+J(\Gamma_1)+2J(\Gamma_2)+J(\Gamma_3)} \begin{pmatrix} J_2 & J_1 & J_3 \\ \Gamma_2 & \Gamma_1 & \Gamma_3 \end{pmatrix} \quad (\text{A1.13})$$

The properties can be used to produce many of the zeros appearing in the tables of Ref. [20]. Any Partition Coefficient containing two or more identical columns cannot exist unless it is even under permutation. Thus coefficients such as;

$$\begin{pmatrix} 3 & 2 & 2 \\ T_2 & T_2 & T_2 \end{pmatrix}, \quad \begin{pmatrix} 4 & 2 & 2 \\ T_1 & T_2 & T_2 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 3 & 3 & 3 \\ T_2 & T_2 & T_2 \end{pmatrix}$$

all vanish. Additional zeros such as $\begin{pmatrix} 3 & 3 & 2 \\ T_2 & T_2 & E \end{pmatrix}$ appear because of the properties of H

or $SU(2)$; in this case the $\begin{pmatrix} 3 & 3 & 2 \\ -2 & 2 & 0 \end{pmatrix}$ $3-j$ symbol is ‘‘accidentally’’ [27] zero.

A.4. Partition Properties

Suitable manipulation of (13) yields;

$$\begin{pmatrix} J_1 & k & J_2 \\ \Gamma_1 & \Gamma_H & \Gamma_2 \end{pmatrix} \langle l^n J_1 || k || l^n J_2 \rangle = \langle l^n J_1 \Gamma_1 || k \Gamma_H || l^n J_2 \Gamma_2 \rangle$$

which can be transformed to;

$$\sum_{\Gamma_1 \Gamma_2} \begin{pmatrix} J_1 & \ell & J_2 \\ \Gamma_1 & \Gamma_H & \Gamma_2 \end{pmatrix}^2 \langle l^n, J_1 \| \ell \| l^n, J_2 \rangle^2 = \sum_{\Gamma_1 \Gamma_2} \langle l^n, J_1, \Gamma_1 \| \ell \Gamma_H \| l^n, J_2, \Gamma_2 \rangle$$

Since $\langle l^n, J_1 \| \ell \| l^n, J_2 \rangle$ is independent of Γ_1 and Γ_3 applying orthonormalization (A1.7) and transposing yields:

$$\langle l^n, J_1 \| \ell \| l^n, J_2 \rangle^2 = \sum_{\Gamma_1 \Gamma_2} \frac{\lambda[\Gamma_H]}{(2k+1)} \langle l^n, J_1, \Gamma_1 \| \ell \Gamma_H \| l^n, J_2, \Gamma_2 \rangle^2 \tag{A1.14}$$

This justifies the name ‘‘Partition Coefficients’’ since it is clear from (A1.14) that these coefficients describe the way a Reduced Matrix Element $\langle l^n, J_1 \| \ell \| l^n, J_2 \rangle$ of $SU(2)$ distributes (partitions) itself over all the possible $\langle l^n, J_1, \Gamma_1 \| \ell \Gamma_H \| l^n, J_2, \Gamma_2 \rangle$ Reduced Matrix Elements of H .

Appendix B. O to T_d Isomorphism

It is well known that when O and T_d are both embedded in an $SU(2)$ or O_h space there exists realization for the eigenvectors of O which are also eigenvectors of T_d [18]. The defining characteristic of this family of realizations is that the Γ_i representations of O do not mix the g or u (even or odd) characters of the O_h ($SU(2)$) representations from which they are subduced.

If these conditions are satisfied, the O vectors are still implicitly g and u in character and the mapping from O to T_d then is [42];

Representation of O	—————>	Representation of T_d	
Γ_{ig}	—————>	Γ_i	
Γ_{iu}	—————>	Γ_i	
Except for;			
A_{1u}	—————>	A_2	(B1.1)
A_{2u}	—————>	A_1	
T_{1u}	—————>	T_2	
T_{2u}	—————>	T_1	

Since, in a ligand field problem, wave functions of odd and even type are never mixed with each other, application of the mapping (B1.1) will allow the Partition Coefficients for T_d to be read from the table of Partition Coefficients of O .

Appendix C. Tables of Partition Coefficients

C.1. Organization

Eqs. (19) and (20) form the basis for the typical use of the Partition Coefficients. As previously discussed in Sect. 6 only limited ranges of values for Γ_H and ℓ are of interest. Further since ℓ is always an integer in all operators of importance, the wave functions are either both integer or both half-integer. For these reasons the table of Partition Coefficients catalogued with respect to Γ_H , ℓ , integer or half-integer wave functions. Further J_1 will always be smaller than J_2 in $\begin{pmatrix} J_1 & \ell & J_2 \\ \Gamma_1 & \Gamma_H & \Gamma_2 \end{pmatrix}$.

Thus if the Partition Coefficient $\begin{pmatrix} 5 & 4 & 4 \\ T_2 & A_1 & T_1 \end{pmatrix}$ is desired, first note that from Eq. (A1.13);

$$(-1)^{5+1} \begin{pmatrix} 5 & 4 & 4 \\ T_1 & A_1 & T_1 \end{pmatrix} = (-1)^{3(5+8+4+1+0+1)} \begin{pmatrix} 4 & 4 & 5 \\ T_1 & A_1 & T_1 \end{pmatrix} = - \begin{pmatrix} 4 & 4 & 5 \\ T_1 & A_1 & T_1 \end{pmatrix}$$

and the Partition Coefficients in standard form will then be found in the table named; $\ell = 4, \Gamma_H = A_1$. The first three columns contain the J_i values and the second three contain the representations in the group O . The value of the square of the Coefficient appears in the last two columns as a rationalized fraction $NUM**2/DEN**2$.

$$\begin{pmatrix} 4 & 4 & 5 \\ T_1 & A_1 & T_1 \end{pmatrix} = - \sqrt{\frac{NUM**2}{DEN**2}} = - \begin{pmatrix} 5 & 4 & 4 \\ T_1 & A_1 & T_1 \end{pmatrix}$$

Note that the sign is associated with the square root and not the values actually given in the tables. Only integer Partition Coefficients are published. Analogous tables for half-integers are available from the authors.

C.2. Characteristics

These tables were obtained by solving Eq. (18) in double precision. The wave functions and 3Γ symbols needed were obtained from a recent set of tabulations [11] which were also derived in double precision. Because they are already well known and thus much easier to cross-check, the four-fold realization of both the subduction coefficients and the 3Γ symbols were employed. The Partition Coefficients were obtained as the rational form of their square using the previously reported techniques [11].

The manuscript tables were formatted and printed directly from computer files to minimize the possibility of transcription errors.

Partition Coefficients

K= 0 ; HAMILTONIAN REP = A1										K= 4 ; HAMILTONIAN REP = A1										K= 6 ; HAMILTONIAN REP = A1									
J1	J2	J3	REP1	REP2	REP3	NUM**2	DEN**2	J1	J2	J3	REP1	REP2	REP3	NUM**2	DEN**2	J1	J2	J3	REP1	REP2	REP3	NUM**2	DEN**2						
0	0	0	A1	A1	A1	1	1	4	4	6	T2	A1	BT2	-1	78	6	6	6	A1	A1	A1	-1	13						
1	0	1	T1	A1	T1	1	1	4	4	7	E	A1	E	-1	39	1	6	5	T1	A1	AT1	-9	572						
2	0	2	E	A1	E	-2	5	4	4	7	T1	A1	AT1	-1	10296	3	6	5	T1	A1	BT1	35	572						
2	0	2	T2	A1	T2	3	5	4	4	7	T1	A1	BT1	-7	312	4	6	6	T2	A1	AT2	-248	1144						
3	0	3	A2	A1	A2	1	7	4	4	7	T2	A1	AT2	-289	6864	5	6	6	T2	A1	BT2	3	520						
3	0	3	T1	A1	T1	3	7	4	4	7	T2	A1	BT2	1	48	6	6	6	T2	A1	BT2	3	520						
3	0	3	T2	A1	T2	3	7	5	4	5	E	A1	E	7	429	7	6	7	E	A1	E	-11	260						
4	0	4	A1	A1	A1	-1	9	5	4	5	AT1	A1	AT1	7	286	8	6	5	T2	A1	T2	3	143						
4	0	4	E	A1	E	-2	9	5	4	5	AT1	A1	BT1	5	286	9	6	5	E	A1	E	-8	143						
4	0	4	T1	A1	T1	1	3	5	4	5	BT1	A1	AT1	5	286	10	6	5	T2	A1	T2	8	143						
4	0	4	T2	A1	T2	1	3	5	4	5	BT1	A1	BT1	-7	286	11	6	5	E	A1	E	-8	143						
5	0	5	E	A1	E	-2	11	5	4	5	T2	A1	T2	14	1287	12	6	5	T2	A1	T2	3	143						
5	0	5	AT1	A1	AT1	3	11	5	4	6	E	A1	E	2	429	13	6	5	T2	A1	T2	3	143						
5	0	5	BT1	A1	BT1	3	11	5	4	6	AT1	A1	T1	35	1144	14	6	5	BT1	A1	T1	-1	1144						
5	0	5	T2	A1	T2	3	11	5	4	6	BT1	A1	T1	-1	1144	15	6	5	T2	A1	T2	3	143						
6	0	6	A1	A1	A1	-1	13	5	4	6	T2	A1	AT2	479	6826	16	6	5	T2	A1	AT2	-1	208						
6	0	6	A2	A1	A2	1	13	5	4	6	T2	A1	BT2	-1	208	17	6	5	E	A1	E	4	221						
6	0	6	E	A1	E	-2	13	5	4	7	E	A1	E	4	221	18	6	5	E	A1	E	4	221						
6	0	6	T1	A1	T1	3	13	5	4	7	AT1	A1	AT1	149	6653	19	6	5	AT1	A1	AT1	-35	1326						
6	0	6	AT2	A1	AT2	3	13	5	4	7	AT1	A1	BT1	-35	1326	20	6	5	AT1	A1	BT1	-7	4862						
6	0	6	BT2	A1	BT2	3	13	5	4	7	BT1	A1	AT1	-7	4862	21	6	5	BT1	A1	BT1	-6	221						
7	0	7	A2	A1	A2	1	15	5	4	7	BT1	A1	BT1	-6	221	22	6	5	T2	A1	AT2	9	9724						
7	0	7	E	A1	E	-2	15	5	4	7	T2	A1	AT2	9	9724	23	6	5	T2	A1	BT2	1	68						
7	0	7	AT1	A1	AT1	1	5	5	4	7	T2	A1	BT2	1	68	24	6	5	A1	A1	A1	147	9724						
7	0	7	BT1	A1	BT1	1	5	6	4	6	A1	A1	A1	147	9724	25	6	5	A2	A1	A2	11	2652						
7	0	7	AT2	A1	AT2	1	5	6	4	6	A2	A1	A2	11	2652	26	6	5	E	A1	E	-225	9091						
7	0	7	BT2	A1	BT2	1	5	6	4	6	E	A1	E	-225	9091	27	6	5	T1	A1	T1	-64	2431						
								6	4	6	T1	A1	T1	-64	2431	28	6	5	AT2	A1	AT2	-179	18001						
								6	4	6	AT2	A1	AT2	-5	3536	29	6	5	AT2	A1	BT2	-5	3536						
								6	4	6	BT2	A1	AT2	-5	3536	30	6	5	BT2	A1	BT2	99	3536						
								6	4	6	BT2	A1	BT2	99	3536	31	6	5	A2	A1	A2	4	153						
								6	4	7	E	A1	E	40	1989	32	6	5	E	A1	E	40	1989						
								6	4	7	T1	A1	AT1	35	4862	33	6	5	T1	A1	AT1	35	4862						
								6	4	7	T1	A1	BT1	-5	1326	34	6	5	T1	A1	BT1	-5	1326						
								6	4	7	AT2	A1	AT2	25	19448	35	6	5	AT2	A1	AT2	25	19448						
								6	4	7	AT2	A1	BT2	1	136	36	6	5	AT2	A1	BT2	1	136						
								6	4	7	BT2	A1	AT2	5	15912	37	6	5	BT2	A1	AT2	5	15912						
								6	4	7	BT2	A1	BT2	55	1224	38	6	5	BT2	A1	BT2	55	1224						
								7	4	7	A2	A1	A2	-104	959310	39	7	4	A2	A1	A2	-104	959310						
								7	4	7	E	A1	E	63	6341	40	7	4	E	A1	E	63	6341						
								7	4	7	AT1	A1	AT1	283	11812	41	7	4	AT1	A1	AT1	283	11812						
								7	4	7	AT1	A1	BT1	336	19349	42	7	4	AT1	A1	BT1	336	19349						
								7	4	7	BT1	A1	AT1	336	19349	43	7	4	BT1	A1	AT1	336	19349						
								7	4	7	BT1	A1	BT1	-189	12682	44	7	4	BT1	A1	BT1	-189	12682						
								7	4	7	AT2	A1	AT2	209	8955	45	7	4	AT2	A1	AT2	209	8955						
								7	4	7	AT2	A1	BT2	52	19349	46	7	4	AT2	A1	BT2	52	19349						
								7	4	7	BT2	A1	AT2	52	19349	47	7	4	BT2	A1	AT2	52	19349						
								7	4	7	BT2	A1	BT2	-133	24033	48	7	4	BT2	A1	BT2	-133	24033						

K= 6 ; HAMILTONIAN REP = A1							
J1	J2	J3	REP1	REP2	REP3	NUM**2	DEN**2
3	6	5	T1	A1	AT1	-7	1144
3	6	5	T1	A1	BT1	-45	1144
3	6	5	T2	A1	T2	-9	286
3	6	6	A2	A1	A2	1	52
3	6	6	T1	A1	T1	-27	1144
3	6	6	T2	A1	AT2	-147	9152
3	6	6	T2	A1	BT2	15	832
3	6	7	A2	A1	A2	4	187
3	6	7	T1	A1	AT1	-63	12155
3	6	7	T1	A1	BT1	-12	1105
3	6	7	T2	A1	AT2	-49	4862
3	6	7	T2	A1	BT2	1	34
4	6	4	A1	A1	A1	40	1287
4	6	4	E	A1	E	-256	6435
4	6	4	T1	A1	T1	1	4290
4	6	4	T2	A1	T2	-5	858
4	6	5	E	A1	E	-3	1430
4	6	5	T1	A1	AT1	-147	2288
4	6	5	T1	A1	BT1	21	11440
4	6	5	T2	A1	T2	-5	572
4	6	6	A1	A1	A1	147	9724
4	6	6	E	A1	E	-135	4862
4	6	6	T1	A1	T1	-105	19448
4	6	6	T2	A1	AT2	1	155584
4	6	6	T2	A1	BT2	196	6845
4	6	7	E	A1	E	2	221
4	6	7	T1	A1	AT1	147	9724
4	6	7	T1	A1	BT1	-7	884
4	6	7	T2	A1	AT2	152	4055
4	6	7	T2	A1	BT2	1	136
5	6	5	E	A1	E	48	12155
5	6	5	AT1	A1	AT1	-10	2431
5	6	5	AT1	A1	BT1	-63	4862
5	6	5	BT1	A1	AT1	-63	4862
5	6	5	BT1	A1	BT1	-72	12155
5	6	5	T2	A1	T2	90	2431
5	6	6	E	A1	E	-70	2431
5	6	6	AT1	A1	T1	152	12165
5	6	6	BT1	A1	T1	105	19448
5	6	6	T2	A1	AT2	42	77792
5	6	6	T2	A1	BT2	105	3536
5	6	7	E	A1	E	-7	16796
5	6	7	AT1	A1	AT1	-945	277134
5	6	7	AT1	A1	BT1	-120	4199
5	6	7	BT1	A1	AT1	267	6967
5	6	7	BT1	A1	BT1	21	33592
5	6	7	T2	A1	AT2	-122	23323
5	6	7	T2	A1	BT2	-7	20672
6	6	6	A1	A1	A1	-40	230945
6	6	6	A2	A1	A2	88	4199
6	6	6	E	A1	E	864	277134
6	6	6	T1	A1	T1	36	277134
6	6	6	AT2	A1	AT2	-65	8331
6	6	6	AT2	A1	BT2	118	5393
6	6	6	BT2	A1	AT2	118	5393
6	6	6	BT2	A1	BT2	33	33592
6	6	7	A2	A1	A2	-1	646
6	6	7	E	A1	E	17	1235
6	6	7	T1	A1	AT1	-173	8608
6	6	7	T1	A1	BT1	-51	19760
6	6	7	AT2	A1	AT2	-186	13475
6	6	7	AT2	A1	BT2	-49	5168
6	6	7	BT2	A1	AT2	-195	16504
6	6	7	BT2	A1	BT2	98	25579
7	6	7	A2	A1	A2	-177	11338
7	6	7	E	A1	E	-88	62965
7	6	7	AT1	A1	AT1	-84	31039
7	6	7	AT1	A1	BT1	21	83980
7	6	7	BT1	A1	AT1	21	83980
7	6	7	BT1	A1	BT1	44	20995
7	6	7	AT2	A1	AT2	78	5219
7	6	7	AT2	A1	BT2	-170	9961
7	6	7	BT2	A1	AT2	-170	9961
7	6	7	BT2	A1	BT2	-133	24033

K= 2 ; HAMILTONIAN REP = E							
J1	J2	J3	REP1	REP2	REP3	NUM**2	DEN**2
0	2	2	A1	E	E	2	5
1	2	1	T1	E	T1	2	5
1	2	2	T1	E	T2	2	5
1	2	3	T1	E	T1	9	35
1	2	3	T1	E	T2	1	7
2	2	2	E	E	E	-8	35
2	2	2	T2	E	T2	6	35
2	2	3	E	E	A2	-1	7
2	2	3	T2	E	T1	3	70
2	2	3	T2	E	T2	-3	14
2	2	4	E	E	A1	-1	15
2	2	4	E	E	E	2	21
2	2	4	T2	E	T1	-1	6
2	2	4	T2	E	T2	1	14
3	2	3	T1	E	T1	4	35
3	2	3	T1	E	T2	-1	7
3	2	3	T2	E	T1	1	7
3	2	4	A2	E	E	-8	105
3	2	4	T1	E	T2	1	7
3	2	4	T2	E	T1	1	15
3	2	4	T2	E	T2	-4	35
3	2	5	A2	E	E	3	55
3	2	5	T1	E	AT1	10	77
3	2	5	T1	E	T2	1	22
3	2	5	T2	E	AT1	-1	154
3	2	5	T2	E	BT1	-9	110
3	2	5	T2	E	T2	9	110
4	2	4	A1	E	E	8	99
4	2	4	E	E	A1	8	99
4	2	4	E	E	E	64	3465
4	2	4	T1	E	T1	-28	165
4	2	4	T1	E	T2	-1	55
4	2	4	T2	E	T1	1	55
4	2	4	T2	E	T2	-16	1155
4	2	5	A1	E	E	1	33
4	2	5	E	E	E	14	165
4	2	5	T1	E	BT1	-6	55
4	2	5	T1	E	T2	1	330
4	2	5	T2	E	AT1	1	22
4	2	5	T2	E	BT1	-7	110
4	2	6	A1	E	E	-20	429
4	2	6	E	E	A1	-3	143
4	2	6	E	E	A2	-7	195
4	2	6	E	E	E	14	429
4	2	6	T1	E	T1	3	143
4	2	6	T1	E	AT2	1	4290
4	2	6	T1	E	BT2	3	26
4	2	6	T2	E	T1	-7	143
4	2	6	T2	E	AT2	56	715
5	2	5	E	E	E	24	715
5	2	5	AT1	E	AT1	10	143
5	2	5	BT1	E	BT1	-18	715
5	2	5	AT1	E	T2	-14	143
5	2	5	BT1	E	T2	-18	715
5	2	5	T2	E	AT1	14	143
5	2	5	T2	E	BT1	18	715
5	2	5	T2	E	T2	-18	715
5	2	6	E	E	A1	-8	143
5	2	6	E	E	A2	-8	455
5	2	6	E	E	E	-16	1001
5	2	6	BT1	E	T1	96	1001
5	2	6	AT1	E	AT2	12	143
5	2	6	BT1	E	AT2	-27	5005
5	2	6	BT1	E	BT2	3	91
5	2	6	T2	E	T1	54	1001
5	2	6	T2	E	AT2	-192	5005
5	2	7	E	E	A2	2	77
5	2	7	E	E	E	-4	91
5	2	7	AT1	E	AT1	63	715
5	2	7	BT1	E	BT1	3	91
5	2	7	AT1	E	AT2	10	715
5	2	7	BT1	E	AT2	1	2002
5	2	7	BT1	E	BT2	1	14
5	2	7	T2	E	AT1	-1	143

; HAMILTONIAN REP = E							; HAMILTONIAN REP = E										
J1	K=	J2	J3	REP1	REP2	REP3	NUM**2	DEN**2	J1	K=	J2	J3	REP1	REP2	REP3	NUM**2	DEN**2
5	2	7		T2	E	BT1	-3	91	3	4	4		T1	E	T1	49	990
5	2	7		T2	E	AT2	72	1001	3	4	4		T1	E	T2	169	2310
6	2	6		A1	E	E	4	715	3	4	4		T2	E	T1	-1	22
6	2	6		A2	E	E	4	91	3	4	4		T2	E	T2	-1	462
6	2	6		E	E	A1	4	715	3	4	5		A2	E	E	8	429
6	2	6		E	E	A2	-4	91	3	4	5		T1	E	AT1	-25	1001
6	2	6		E	E	E	-288	5065	3	4	5		T1	E	BT1	-49	715
6	2	6		T1	E	T1	-6	5065	3	4	5		T1	E	T2	1	715
6	2	6		T1	E	AT2	-27	1001	3	4	5		T2	E	AT1	80	1001
6	2	6		T1	E	BT2	-3	455	3	4	5		T2	E	BT1	-4	143
6	2	6		AT2	E	T1	27	1001	3	4	5		T2	E	T2	-1	1287
6	2	6		BT2	E	T1	3	455	3	4	6		A2	E	E	16	429
6	2	6		AT2	E	AT2	-30	1001	3	4	6		T1	E	T1	-5	143
6	2	6		BT2	E	BT2	66	455	3	4	6		T1	E	AT2	8	143
6	2	7		A1	E	E	11	260	3	4	6		T2	E	T1	-1	143
6	2	7		A2	E	E	-9	364	3	4	6		T2	E	AT2	-125	2574
6	2	7		E	E	A2	-1	35	3	4	6		T2	E	BT2	1	26
6	2	7		E	E	E	11	910	3	4	7		A2	E	E	2	65
6	2	7		T1	E	BT1	-33	455	3	4	7		T1	E	AT1	-175	5148
6	2	7		T1	E	AT2	5	728	3	4	7		T1	E	BT1	1	156
6	2	7		T1	E	BT2	-11	280	3	4	7		T1	E	AT2	8	143
6	2	7		AT2	E	AT1	1	26	3	4	7		T2	E	AT1	-7	715
6	2	7		AT2	E	BT1	-33	728	3	4	7		T2	E	BT1	-3	65
6	2	7		BT2	E	BT1	3	3640	3	4	7		T2	E	AT2	81	5720
6	2	7		AT2	E	AT2	-9	364	3	4	7		T2	E	BT2	-1	40
6	2	7		BT2	E	BT2	9	140	4	4	4		A1	E	E	-4	3861
7	2	7		A2	E	E	-44	1785	4	4	4		E	E	A1	-4	3861
7	2	7		E	E	A2	-44	1785	4	4	4		E	E	E	357	3769
7	2	7		E	E	E	-32	23205	4	4	4		T1	E	T1	-35	2574
7	2	7		AT1	E	AT1	56	1105	4	4	4		T1	E	T2	15	286
7	2	7		BT1	E	BT1	8	7735	4	4	4		T2	E	T1	-15	286
7	2	7		AT1	E	AT2	-81	1105	4	4	4		T2	E	T2	118	17009
7	2	7		BT1	E	AT2	-165	6188	4	4	5		A1	E	E	8	143
7	2	7		BT1	E	BT2	-27	2380	4	4	5		T1	E	AT1	7	1287
7	2	7		AT2	E	AT1	81	1105	4	4	5		T1	E	BT1	-5	143
7	2	7		AT2	E	BT1	165	6188	4	4	5		T1	E	T2	-5	143
7	2	7		BT2	E	BT1	27	2380	4	4	5		T2	E	AT1	-4	429
7	2	7		AT2	E	AT2	-242	7735	4	4	5		T2	E	T2	35	429
7	2	7		BT2	E	BT2	26	595	4	4	6		A1	E	E	16	1287
									4	4	6		E	E	A1	-256	6435
									4	4	6		E	E	E	-224	6A35
									4	4	6		T1	E	T1	5	143
									4	4	6		T1	E	AT2	-2	143
									4	4	6		T1	E	BT2	-2	65
									4	4	6		T2	E	T1	-21	715
									4	4	6		T2	E	AT2	7	858
									4	4	6		T2	E	BT2	7	390
									4	4	7		A1	E	E	-1	39
									4	4	7		E	E	A2	7	165
									4	4	7		T1	E	AT1	-7	51480
									4	4	7		T1	E	BT1	5	312
									4	4	7		T1	E	AT2	9	2860
									4	4	7		T1	E	BT2	1	20
									4	4	7		T2	E	AT1	98	2145
									4	4	7		T2	E	AT2	-120	12887
									4	4	7		T2	E	BT2	-7	240
									5	4	5		E	E	E	-10	429
									5	4	5		AT1	E	AT1	-5	286
									5	4	5		AT1	E	BT1	7	286
									5	4	5		BT1	E	AT1	7	286
									5	4	5		BT1	E	BT1	5	286
									5	4	5		AT1	E	T2	-7	286
									5	4	5		BT1	E	T2	5	286
									5	4	5		T2	E	AT1	7	286
									5	4	5		T2	E	BT1	-5	286
									5	4	5		T2	E	T2	-40	1287
									5	4	6		E	E	A1	-3	1430
									5	4	6		E	E	A2	25	546
									5	4	6		E	E	E	11	1365
									5	4	6		AT1	E	T1	49	1144
									5	4	6		BT1	E	T1	5	8008
									5	4	6		AT1	E	AT2	5	143
									5	4	6		BT1	E	AT2	11	364
									5	4	6		BT1	E	BT2	-81	1820
									5	4	6		T2	E	T1	32	5005

K= 4						; HAMILTONIAN REP = E	
J1	J2	J3	REP1	REP2	REP3	NUM**2	DEN**2
5	4	6	T2	E	AT2	1	144144
5	4	6	T2	E	BT2	7	1040
5	4	7	E	E	A2	-16	6545
5	4	7	E	E	F	-40	1547
5	4	7	AT1	E	AT1	-131	8189
5	4	7	AT1	E	BT1	-49	1326
5	4	7	BT1	E	AT1	-49	24310
5	4	7	BT1	E	BT1	30	1547
5	4	7	AT1	E	AT2	-1	2431
5	4	7	BT1	E	AT2	-205	10634
5	4	7	BT1	E	BT2	9	2300
5	4	7	T2	E	AT1	358	8499
5	4	7	T2	E	BT1	-30	1547
5	4	7	T2	E	AT2	-200	14297
5	4	7	T2	E	BT2	-7	340
6	4	6	A1	E	E	-135	4862
6	4	6	A2	E	E	121	9282
6	4	6	E	E	A1	-135	4862
6	4	6	E	E	A2	-121	9282
6	4	6	E	E	E	-20	51051
6	4	6	T1	E	T1	247	13135
6	4	6	T1	E	AT2	1058	272272
6	4	6	T1	E	BT2	181	5531
6	4	6	AT2	E	T1	-1058	272272
6	4	6	BT2	E	T1	-181	5531
6	4	6	AT2	E	AT2	10798	445416
6	4	6	AT2	E	BT2	7	3536
6	4	6	BT2	E	AT2	7	3536
6	4	6	BT2	E	BT2	246	12301
6	4	7	A1	E	E	-2	221
6	4	7	A2	E	E	-22	69615
6	4	7	E	E	A2	-128	11781
6	4	7	E	E	E	227	6530
6	4	7	T1	E	AT1	49	4862
6	4	7	T1	E	BT1	25	9282
6	4	7	T1	E	AT2	-296	13953
6	4	7	T1	E	BT2	1	119
6	4	7	AT2	E	AT1	-9	12155
6	4	7	AT2	E	BT1	-158	13467
6	4	7	BT2	E	BT1	-184	12421
6	4	7	AT2	E	AT2	347	6341
6	4	7	AT2	E	BT2	-7	680
6	4	7	BT2	E	AT2	-7	15912
6	4	7	BT2	E	BT2	243	7571
7	4	7	A2	E	E	34	3591
7	4	7	E	E	A2	34	3591
7	4	7	E	E	E	-90	6341
7	4	7	AT1	E	AT1	-132	10753
7	4	7	AT1	E	BT1	233	9584
7	4	7	BT1	E	AT1	233	9584
7	4	7	BT1	E	BT1	118	11085
7	4	7	AT1	E	AT2	-243	10162
7	4	7	BT1	E	AT2	75	235144
7	4	7	BT1	E	BT2	568	23157
7	4	7	AT2	E	AT1	243	10162
7	4	7	AT2	E	BT1	-75	235144
7	4	7	BT2	E	BT1	-568	23157
7	4	7	AT2	E	AT2	-121	14149
7	4	7	AT2	E	BT2	-175	46512
7	4	7	BT2	E	AT2	-175	46512
7	4	7	BT2	E	BT2	-95	24033

K= 6						; HAMILTONIAN REP = E	
J1	J2	J3	REP1	REP2	REP3	NUM**2	DEN**2
1	6	7	T1	E	BT2	11	560
2	6	4	E	E	A1	-20	429
2	6	4	E	E	E	14	429
2	6	4	T2	E	T1	32	429
2	6	5	E	E	E	-16	1001
2	6	5	T2	E	AT1	-15	572
2	6	5	T2	E	BT1	-21	572
2	6	5	T2	E	T2	-75	1001
2	6	6	E	E	A1	4	715
2	6	6	E	E	A2	4	91
2	6	6	E	E	E	-288	5005
2	6	6	T2	E	T1	3	5005
2	6	6	T2	E	AT2	33	728
2	6	6	T2	E	BT2	-3	3640
2	6	7	E	E	A2	-1	35
2	6	7	E	E	E	-11	910
2	6	7	T2	E	AT1	5	416
2	6	7	T2	E	BT1	212	10393
2	6	7	T2	E	AT2	-148	1951
2	6	7	T2	E	BT2	-11	2240
3	6	3	T1	E	T1	25	286
3	6	3	T1	E	T2	5	286
3	6	3	T2	E	T1	-5	286
3	6	3	T2	E	T2	-9	286
3	6	4	A2	E	E	16	429
3	6	4	T1	E	T1	-15	2002
3	6	4	T1	E	T2	5	286
3	6	4	T2	E	T1	361	6006
3	6	4	T2	E	T2	9	286
3	6	5	A2	E	E	-48	1001
3	6	5	T1	E	AT1	49	1144
3	6	5	T1	E	BT1	-45	8008
3	6	5	T1	E	T2	5	2002
3	6	5	T2	E	AT1	5	1144
3	6	5	T2	E	BT1	-81	8008
3	6	5	T2	E	T2	-81	2002
3	6	6	A2	E	E	-5	2002
3	6	6	T1	E	T1	-27	8008
3	6	6	T1	E	AT2	105	9152
3	6	6	T1	E	BT2	-363	5824
3	6	6	T2	E	T1	-375	8008
3	6	6	T2	E	AT2	125	5046
3	6	6	T2	E	BT2	-15	5824
3	6	7	A2	E	E	8	1547
3	6	7	T1	E	AT1	499	11273
3	6	7	T1	E	BT1	-12	7735
3	6	7	T1	E	AT2	97	23955
3	6	7	T1	E	BT2	-498	8707
3	6	7	T2	E	AT1	137	8526
3	6	7	T2	E	BT1	27	24752
3	6	7	T2	E	AT2	171	6056
3	6	7	T2	E	BT2	-1	238
4	6	4	A1	E	E	16	1287
4	6	4	E	E	A1	16	1287
4	6	4	E	E	E	-224	6435
4	6	4	T1	E	T1	-7	4290
4	6	4	T1	E	T2	9	1430
4	6	4	T2	E	T1	-9	1430
4	6	4	T2	E	T2	343	4290
4	6	5	A1	E	E	2	429
4	6	5	E	E	E	11	1365
4	6	5	T1	E	AT1	-21	2288
4	6	5	T1	E	BT1	-147	11440
4	6	5	T1	E	T2	289	8580
4	6	5	T2	E	AT1	-25	2288
4	6	5	T2	E	BT1	77	1040
4	6	5	T2	E	T2	-9	20020
4	6	6	A1	E	E	-225	9091
4	6	6	E	E	A1	-135	4862
4	6	6	E	E	A2	121	9282
4	6	6	E	E	E	-20	51051
4	6	6	T1	E	T1	137	3625
4	6	6	T1	E	AT2	71	24207
4	6	6	T1	E	BT2	15	14144
4	6	6	T2	E	T1	185	13953

K= 6						K= 6						K= 6						K= 2						
J1	J2	J3	HAMILTONIAN			REP =	E	J1	J2	J3	HAMILTONIAN			REP =	E	J1	J2	J3	HAMILTONIAN			REP =	T2	E
			REP1	REP2	REP3	NUM**2	DEN**2				REP1	REP2	REP3	NUM**2	DEN**2				REP1	REP2	REP3	NUM**2	DEN**2	
4	6	6	T2	E	A2	-232	8665	7	6	7	A2	E	E	56	4845				A2	E	E	56	4845	
4	6	6	T2	E	BT2	-28	6845	7	6	7	E	E	A2	56	4845				E	E	A2	56	4845	
4	6	7	A1	E	E	-40	1989	7	6	7	E	E	E	153	7822				E	E	E	153	7822	
4	6	7	E	E	A2	-128	11781	7	6	7	AT1	E	AT1	207	10927				AT1	E	AT1	207	10927	
4	6	7	E	E	E	-227	6530	7	6	7	AT1	E	BT1	3	83980				AT1	E	BT1	3	83980	
4	6	7	T1	E	AT1	21	9724	7	6	7	BT1	E	AT1	3	83980				BT1	E	AT1	3	83980	
4	6	7	T1	E	BT1	49	884	7	6	7	BT1	E	BT1	-151	10293				BT1	E	BT1	-151	10293	
4	6	7	T1	E	A2	-184	15287	7	6	7	AT1	E	A2	-1125	369512				AT1	E	A2	-1125	369512	
4	6	7	T1	E	BT2	-3	544	7	6	7	AT1	E	BT2	-121	12920				AT1	E	BT2	-121	12920	
4	6	7	T2	E	AT1	-18	77792	7	6	7	BT1	E	A2	-65	14441				BT1	E	A2	-65	14441	
4	6	7	T2	E	BT1	-35	21479	7	6	7	AT2	E	AT1	1125	369512				AT2	E	AT1	1125	369512	
4	6	7	T2	E	A2	224	22275	7	6	7	AT2	E	BT1	65	14441				AT2	E	BT1	65	14441	
4	6	7	T2	E	BT2	-1	952	7	6	7	BT2	E	AT1	121	12920				BT2	E	AT1	121	12920	
5	6	5	E	E	E	-205	3708	7	6	7	AT2	E	A2	-35	739024				AT2	E	A2	-35	739024	
5	6	5	AT1	E	AT1	70	2431	7	6	7	AT2	E	BT2	63	25840				AT2	E	BT2	63	25840	
5	6	5	AT1	E	BT1	-9	4862	7	6	7	BT2	E	AT2	63	25840				BT2	E	AT2	63	25840	
5	6	5	BT1	E	AT1	-9	4862	7	6	7	BT2	E	BT2	-296	7641				BT2	E	BT2	-296	7641	
5	6	5	BT1	E	BT1	205	4944																	
5	6	5	AT1	E	T2	-25	19448																	
5	6	5	BT1	E	T2	-567.	97240																	
5	6	5	T2	E	AT1	25	19448	J1	J2	J3	HAMILTONIAN			REP =	T2	DEN**2								
5	6	5	T2	E	BT1	567	97240	0	2	2	A1	T2	T2	3	5				A1	T2	T2	3	5	
5	6	5	T2	E	T2	126	12155	1	2	1	T1	T2	T1	3	5				T1	T2	T1	3	5	
5	6	6	E	E	A1	70	2431	1	2	2	T1	T2	E	2	5				T1	T2	E	2	5	
5	6	6	E	E	A2	-2	221	1	2	2	T1	T2	T2	1	5				T1	T2	T2	1	5	
5	6	6	AT1	E	T1	486	272272	1	2	3	T1	T2	A2	1	7				T1	T2	A2	1	7	
5	6	6	BT1	E	T1	-137	3625	1	2	3	T1	T2	T1	-6	35				T1	T2	T1	-6	35	
5	6	6	AT1	E	A2	116	12459	1	2	3	T1	T2	T2	-2	7				T1	T2	T2	-2	7	
5	6	6	AT1	E	BT2	315	21479	2	2	2	E	T2	T2	-6	35				E	T2	T2	-6	35	
5	6	6	BT1	E	A2	33	3536	2	2	2	T2	T2	E	6	35				T2	T2	E	6	35	
5	6	6	BT1	E	BT2	15	3536	2	2	2	T2	T2	T2	9	35				T2	T2	T2	9	35	
5	6	6	T2	E	T1	30	2431	2	2	3	E	T2	T1	3	70				E	T2	T1	3	70	
5	6	6	T2	E	A2	-51	2288	2	2	3	E	T2	T2	-3	14				E	T2	T2	-3	14	
5	6	6	T2	E	BT2	-15	3536	2	2	3	T2	T2	T1	12	35				T2	T2	T1	12	35	
5	6	7	E	E	A2	-9	3553	2	2	4	E	T2	T1	1	6				E	T2	T1	1	6	
5	6	7	E	E	E	49	8398	2	2	4	E	T2	T2	-1	14				E	T2	T2	-1	14	
5	6	7	AT1	E	AT1	6615	277134	2	2	4	T2	T2	A1	-2	45				T2	T2	A1	-2	45	
5	6	7	AT1	E	BT1	-103	25229	2	2	4	T2	T2	E	8	63				T2	T2	E	8	63	
5	6	7	BT1	E	AT1	119	21736	2	2	4	T2	T2	T2	4	21				T2	T2	T2	4	21	
5	6	7	BT1	E	BT1	-118	26965	3	2	3	A2	T2	T1	-1	7				A2	T2	T1	-1	7	
5	6	7	AT1	E	A2	-174	8890185	3	2	3	T1	T2	A2	-1	7				T1	T2	A2	-1	7	
5	6	7	AT1	E	BT2	172	4571	3	2	3	T1	T2	T1	-3	280				T1	T2	T1	-3	280	
5	6	7	BT1	E	A2	135	10283	3	2	3	T1	T2	T2	-1	56				T1	T2	T2	-1	56	
5	6	7	BT1	E	BT2	-97	11865	3	2	3	T2	T2	T1	-1	56				T2	T2	T1	-1	56	
5	6	7	T2	E	AT1	105	13189	3	2	3	T2	T2	T2	15	56				T2	T2	T2	15	56	
5	6	7	T2	E	BT1	-45	1199	3	2	4	A2	T2	T1	-1	15				A2	T2	T1	-1	15	
5	6	7	T2	E	A2	-62	19479	3	2	4	T1	T2	E	1	7				T1	T2	E	1	7	
5	6	7	T2	E	BT2	1	20672	3	2	4	T1	T2	T1	-1	8				T1	T2	T1	-1	8	
6	6	6	A1	E	E	864	277134	3	2	4	T1	T2	T2	-1	56				T1	T2	T2	-1	56	
6	6	6	E	E	A1	864	277134	3	2	4	T2	T2	A1	-1	9				T2	T2	A1	-1	9	
6	6	6	E	E	E	-209	10774	3	2	4	T2	T2	E	1	315				T2	T2	E	1	315	
6	6	6	T1	E	T1	-252	277134	3	2	4	T2	T2	T1	-3	40				T2	T2	T1	-3	40	
6	6	6	T1	E	A2	209	5090	3	2	4	T2	T2	T2	-7	120				T2	T2	T2	-7	120	
6	6	6	T1	E	BT2	-131	16764	3	2	5	A2	T2	AT1	1	154				A2	T2	AT1	1	154	
6	6	6	AT2	E	T1	-209	5090	3	2	5	A2	T2	BT1	-9	110				A2	T2	BT1	-9	110	
6	6	6	BT2	E	T1	131	16764	3	2	5	T1	T2	E	1	22				T1	T2	E	1	22	
6	6	6	AT2	E	A2	148	9011	3	2	5	T1	T2	AT1	15	308				T1	T2	AT1	15	308	
6	6	6	AT2	E	BT2	-92	29433	3	2	5	T1	T2	BT1	3	44				T1	T2	BT1	3	44	
6	6	6	BT2	E	A2	-92	29433	3	2	5	T1	T2	T2	11	11				T1	T2	T2	11	11	
6	6	6	BT2	E	BT2	131	19080	3	2	5	T2	T2	E	-9	110				T2	T2	E	-9	110	
6	6	7	A1	E	E	-17	1235	3	2	5	T2	T2	AT1	-25	308				T2	T2	AT1	-25	308	
6	6	7	A2	E	E	-77	4199	3	2	5	T2	T2	BT1	9	220				T2	T2	BT1	9	220	
6	6	7	E	E	A2	-285	14761	3	2	5	T2	T2	T2	3	55				T2	T2	T2	3	55	
6	6	7	T1	E	AT1	-2203	767306	4	2	4	A1	T2	T2	-1	33				A1	T2	T2	-1	33	
6	6	7	T1	E	BT1	317	17546	4	2	4	E	T2	T1	-1	55				E	T2	T1	-1	55	
6	6	7	T1	E	A2	45	13648	4	2	4	E	T2	T2	-11	105				E	T2	T2	-11	105	
6	6	7	T1	E	BT2	35	10336	4	2	4	T1	T2	E	1	55				T1	T2	E	1	55	
6	6	7	AT2	E	AT1	-650	227392	4	2	4	T1	T2	T1	7	440				T1	T2	T1	7	440	
6	6	7	AT2	E	BT1	7623	403104	4	2	4	T1	T2	T2	-49	440				T1	T2	T2	-49	440	
6	6	7	BT2	E	AT1	1089	671840	4	2	4	T2	T2	A1	1	33				T2	T2	A1	1	33	
6	6	7	BT2	E	BT1	128	14891	4	2	4	T2	T2	E	11	105				T2	T2	E	11	105	
6	6	7	AT2	E	A2	-203	15655	4	2	4	T2	T2	T1	49	440				T2	T2	T1	49	440	
6	6	7	AT2	E	BT2	7	5168	4	2	4	T2	T2	T2	-169	3080				T2	T2	T2	-169	3080	
6	6	7	BT2	E	AT2	31	18366	4	2	5	A1	T2	T2	-8	99				A1	T2	T2	-8	99	
6	6	7	BT2	E	BT2	296	11037	4	2	5	E	T2	AT1	1	22				E	T2	AT1	1	22	

HAMILTONIAN REP = T2							HAMILTONIAN REP = T2										
J1	K=	J2	J3	REP1	REP2	REP3	NUM**2	DEN**2	J1	K=	J2	J3	REP1	REP2	REP3	NUM**2	DEN**2
5	2	7		T2	T2	BT2	-3	112	4	2	5		E	T2	BT1	7	110
6	2	6		A1	T2	AT2	-75	1144	4	2	5		E	T2	T2	-14	495
6	2	6		A1	T2	BT2	-3	520	4	2	5		T1	T2	E	-1	330
6	2	6		A2	T2	T1	3	91	4	2	5		T1	T2	AT1	-7	44
6	2	6		E	T2	T1	-3	5005	4	2	5		T1	T2	BT1	1	220
6	2	6		E	T2	AT2	-33	728	4	2	5		T1	T2	T2	3	55
6	2	6		E	T2	BT2	3	3640	4	2	5		T2	T2	E	-7	110
6	2	6		T1	T2	A2	-3	91	4	2	5		T2	T2	AT1	1	44
6	2	6		T1	T2	E	3	5005	4	2	5		T2	T2	BT1	7	220
6	2	6		T1	T2	T1	439	3379	4	2	5		T2	T2	T2	-7	165
6	2	6		T1	T2	AT2	-116	15291	4	2	6		A1	T2	AT2	-13	792
6	2	6		T1	T2	BT2	-245	9827	4	2	6		A1	T2	BT2	5	104
6	2	6		AT2	T2	A1	75	1144	4	2	6		E	T2	T1	7	143
6	2	6		BT2	T2	A1	3	520	4	2	6		E	T2	AT2	-77	4680
6	2	6		AT2	T2	E	33	728	4	2	6		E	T2	BT2	-7	104
6	2	6		BT2	T2	E	-3	3640	4	2	6		T1	T2	A2	8	195
6	2	6		AT2	T2	T1	-116	15291	4	2	6		T1	T2	E	32	429
6	2	6		BT2	T2	T1	245	9827	4	2	6		T1	T2	T1	2	143
6	2	6		AT2	T2	AT2	-88	10227	4	2	6		T1	T2	AT2	-48	715
6	2	6		AT2	T2	BT2	329	7038	4	2	6		T2	T2	A1	8	143
6	2	6		BT2	T2	AT2	-329	7038	4	2	6		T2	T2	T1	14	143
6	2	6		BT2	T2	BT2	-23	27061	4	2	6		T2	T2	AT2	112	2145
6	2	7		A1	T2	AT2	-1	4160	5	2	5		E	T2	AT1	-14	143
6	2	7		A1	T2	BT2	11	320	5	2	5		E	T2	BT1	18	715
6	2	7		A2	T2	AT1	11	416	5	2	5		E	T2	T2	18	715
6	2	7		A2	T2	BT1	75	2912	5	2	5		AT1	T2	E	-14	143
6	2	7		E	T2	AT1	5	416	5	2	5		BT1	T2	E	18	715
6	2	7		E	T2	BT1	212	10393	5	2	5		AT1	T2	AT1	15	9152
6	2	7		E	T2	AT2	-148	1951	5	2	5		AT1	T2	BT1	21	9152
6	2	7		E	T2	BT2	-11	2240	5	2	5		BT1	T2	AT1	21	9152
6	2	7		T1	T2	A2	4	105	5	2	5		BT1	T2	BT1	351	3520
6	2	7		T1	T2	E	-11	1365	5	2	5		AT1	T2	T2	7	2288
6	2	7		T1	T2	AT1	3	130	5	2	5		BT1	T2	T2	-99	1040
6	2	7		T1	T2	BT1	-11	910	5	2	5		T2	T2	E	-18	715
6	2	7		T1	T2	AT2	81	7280	5	2	5		T2	T2	AT1	7	2288
6	2	7		T1	T2	BT2	-11	560	5	2	5		T2	T2	BT1	-99	1040
6	2	7		AT2	T2	E	33	728	5	2	5		T2	T2	T2	3	2860
6	2	7		BT2	T2	E	-3	3640	5	2	6		E	T2	T1	54	1001
6	2	7		AT2	T2	AT1	1	208	5	2	6		E	T2	AT2	-27	5005
6	2	7		AT2	T2	BT1	33	1456	5	2	6		E	T2	BT2	3	91
6	2	7		BT2	T2	AT1	-99	1040	5	2	6		AT1	T2	A2	3	52
6	2	7		BT2	T2	BT1	-3	7280	5	2	6		BT1	T2	A2	-3	1820
6	2	7		AT2	T2	AT2	-21	1664	5	2	6		AT1	T2	E	15	572
6	2	7		AT2	T2	BT2	-33	896	5	2	6		BT1	T2	E	21	572
6	2	7		BT2	T2	AT2	-152	2217	5	2	6		AT1	T2	T1	45	2288
6	2	7		BT2	T2	BT2	3	4480	5	2	6		BT1	T2	T1	-9	16016
7	2	7		A2	T2	AT1	-27	680	5	2	6		AT1	T2	AT2	75	18304
7	2	7		A2	T2	BT1	11	4760	5	2	6		AT1	T2	BT2	135	1664
7	2	7		E	T2	AT1	297	8840	5	2	6		BT1	T2	AT2	-371	3985
7	2	7		E	T2	BT1	-473	13250	5	2	6		BT1	T2	BT2	75	11648
7	2	7		E	T2	AT2	-165	6188	5	2	6		T2	T2	A1	3	143
7	2	7		E	T2	BT2	27	2380	5	2	6		T2	T2	E	-75	1001
7	2	7		AT1	T2	A2	-27	680	5	2	6		T2	T2	T1	-27	4004
7	2	7		BT1	T2	A2	11	4760	5	2	6		T2	T2	AT2	-81	160160
7	2	7		AT1	T2	E	297	8840	5	2	6		T2	T2	BT2	-225	2912
7	2	7		BT1	T2	E	-473	13250	5	2	7		E	T2	AT1	1	143
7	2	7		AT1	T2	AT1	-105	226304	5	2	7		E	T2	BT1	-3	91
7	2	7		AT1	T2	BT1	-18	22859	5	2	7		E	T2	AT2	1	2002
7	2	7		BT1	T2	AT1	-18	22859	5	2	7		E	T2	BT2	-1	14
7	2	7		BT1	T2	BT1	62	1831	5	2	7		AT1	T2	A2	3	220
7	2	7		AT1	T2	AT2	-405	452608	5	2	7		BT1	T2	A2	25	924
7	2	7		AT1	T2	BT2	-13	22859	5	2	7		AT1	T2	E	-3	260
7	2	7		BT1	T2	AT2	103	17602	5	2	7		BT1	T2	E	7	156
7	2	7		BT1	T2	BT2	-411	4985	5	2	7		AT1	T2	AT1	-105	4576
7	2	7		AT2	T2	E	165	6188	5	2	7		AT1	T2	BT1	-81	2080
7	2	7		BT2	T2	E	-27	2380	5	2	7		BT1	T2	AT1	-147	4576
7	2	7		AT2	T2	AT1	405	452608	5	2	7		BT1	T2	BT1	13	224
7	2	7		AT2	T2	BT1	-103	17602	5	2	7		AT1	T2	AT2	-323	7299
7	2	7		BT2	T2	AT1	13	22859	5	2	7		AT1	T2	BT2	-9	320
7	2	7		BT2	T2	BT1	411	4985	5	2	7		BT1	T2	AT2	-59	16799
7	2	7		AT2	T2	AT2	-105	905216	5	2	7		BT1	T2	BT2	-1	448
7	2	7		AT2	T2	BT2	160	4543	5	2	7		T2	T2	E	3	91
7	2	7		BT2	T2	AT2	160	4543	5	2	7		T2	T2	AT1	-49	1144
7	2	7		BT2	T2	BT2	419	27246	5	2	7		T2	T2	BT1	-3	728
5	2	7		T2	T2	AT2			5	2	7		T2	T2	AT2	332	6133

K= 4 ; HAMILTONIAN REP = T2								K= 4 ; HAMILTONIAN REP = T2							
J1	J2	J3	REP1	REP2	REP3	NUM**2	DEN**2	J1	J2	J3	REP1	REP2	REP3	NUM**2	DEN**2
0	4	4	A1	T2	T2	-1	3	3	4	7	T1	T2	AT2	1	2288
1	4	3	T1	T2	A2	1	7	3	4	7	T1	T2	BT2	-1	16
1	4	3	T1	T2	T1	5	168	3	4	7	T2	T2	E	3	65
1	4	3	T1	T2	T2	-9	56	3	4	7	T2	T2	AT1	63	5720
1	4	4	T1	T2	E	1	15	3	4	7	T2	T2	BT1	-27	520
1	4	4	T1	T2	T1	-7	120	3	4	7	T2	T2	AT2	3	11440
1	4	4	T1	T2	T2	5	24	3	4	7	T2	T2	BT2	-3	80
1	4	5	T1	T2	E	7	55	4	4	4	A1	T2	T2	13	198
1	4	5	T1	T2	AT1	-3	66	4	4	4	E	T2	T1	15	286
1	4	5	T1	T2	BT1	21	110	4	4	4	E	T2	T2	-118	17009
2	4	2	E	T2	T2	-1	14	4	4	4	T1	T2	E	-15	286
2	4	2	T2	T2	E	1	14	4	4	4	T1	T2	T1	-35	429
2	4	2	T2	T2	T2	4	21	4	4	4	T2	T2	A1	-13	198
2	4	3	E	T2	T1	-1	7	4	4	4	T2	T2	E	118	17009
2	4	3	E	T2	T2	4	35	4	4	4	T2	T2	T2	5	3003
2	4	3	T2	T2	T1	-1	56	4	4	5	A1	T2	T2	1	429
2	4	3	T2	T2	T2	7	120	4	4	5	E	T2	AT1	-4	429
2	4	4	E	T2	T1	-1	55	4	4	5	E	T2	T2	35	429
2	4	4	E	T2	T2	16	1155	4	4	5	T1	T2	E	5	143
2	4	4	T2	T2	A1	1	33	4	4	5	T1	T2	AT1	7	13728
2	4	4	T2	T2	E	11	105	4	4	5	T1	T2	BT1	-135	4576
2	4	4	T2	T2	T1	49	440	4	4	5	T1	T2	T2	-5	286
2	4	4	T2	T2	T2	169	3080	4	4	5	T2	T2	AT1	-391	2903
2	4	5	E	T2	AT1	1	22	4	4	5	T2	T2	BT1	-105	4576
2	4	5	E	T2	BT1	-7	110	4	4	6	A1	T2	AT2	5	858
2	4	5	E	T2	T2	-7	110	4	4	6	A1	T2	BT2	1	78
2	4	5	T2	T2	E	7	110	4	4	6	E	T2	T1	21	715
2	4	5	T2	T2	AT1	-1	44	4	4	6	E	T2	AT2	-7	858
2	4	5	T2	T2	BT1	-7	220	4	4	6	E	T2	BT2	-7	390
2	4	5	T2	T2	T2	-7	165	4	4	6	T1	T2	A2	-1	26
2	4	6	E	T2	T1	7	143	4	4	6	T1	T2	E	-9	1430
2	4	6	E	T2	AT2	-56	715	4	4	6	T1	T2	T1	-3	1430
2	4	6	T2	T2	A1	8	143	4	4	6	T1	T2	AT2	11	832
2	4	6	T2	T2	T1	14	143	4	4	6	T1	T2	BT2	-49	4160
2	4	6	T2	T2	AT2	-112	2145	4	4	6	T2	T2	A1	-5	858
3	4	3	A2	T2	T1	-1	154	4	4	6	T2	T2	E	343	4290
3	4	3	T1	T2	A2	-1	154	4	4	6	T2	T2	AT2	175	9152
3	4	3	T1	T2	T1	-15	77	4	4	6	T2	T2	BT2	343	4160
3	4	3	T1	T2	T2	4	77	4	4	7	A1	T2	AT2	-289	6864
3	4	3	T2	T2	T1	4	77	4	4	7	A1	T2	BT2	1	48
3	4	3	T2	T2	T2	-5	231	4	4	7	E	T2	AT1	98	2145
3	4	4	A2	T2	T1	1	22	4	4	7	E	T2	AT2	-120	12007
3	4	4	T1	T2	E	169	2310	4	4	7	E	T2	BT2	-7	240
3	4	4	T1	T2	T1	-4	165	4	4	7	T1	T2	A2	-2	165
3	4	4	T1	T2	T2	5	231	4	4	7	T1	T2	E	8	195
3	4	4	T2	T2	A1	-5	66	4	4	7	T1	T2	AT1	-35	1716
3	4	4	T2	T2	E	1	462	4	4	7	T1	T2	BT1	-9	260
3	4	4	T2	T2	T1	-1	11	4	4	7	T1	T2	AT2	32	715
3	4	5	A2	T2	AT1	-80	1001	4	4	7	T2	T2	AT1	49	8580
3	4	5	A2	T2	BT1	-4	143	4	4	7	T2	T2	BT1	-7	260
3	4	5	T1	T2	E	1	715	5	4	5	E	T2	AT1	-7	286
3	4	5	T1	T2	AT1	166	6133	5	4	5	E	T2	BT1	-5	286
3	4	5	T1	T2	BT1	-33	2080	5	4	5	E	T2	T2	5	286
3	4	5	T1	T2	T2	5	286	5	4	5	AT1	T2	E	-7	286
3	4	5	T2	T2	E	4	143	5	4	5	BT1	T2	E	-5	286
3	4	5	T2	T2	AT1	-55	2912	5	4	5	AT1	T2	AT1	15	572
3	4	5	T2	T2	BT1	1	4576	5	4	5	AT1	T2	BT1	-21	572
3	4	5	T2	T2	T2	-50	429	5	4	5	BT1	T2	AT1	-21	572
3	4	6	A2	T2	T1	1	143	5	4	5	BT1	T2	BT1	-15	572
3	4	6	T1	T2	A2	1	26	5	4	5	AT1	T2	T2	7	572
3	4	6	T1	T2	E	5	286	5	4	5	BT1	T2	T2	-5	572
3	4	6	T1	T2	T1	-15	286	5	4	5	T2	T2	E	-5	286
3	4	6	T1	T2	AT2	-307	7783	5	4	5	T2	T2	AT1	-7	572
3	4	6	T1	T2	BT2	45	832	5	4	5	T2	T2	BT1	5	572
3	4	6	T2	T2	A1	-7	286	5	4	5	T2	T2	T2	-20	429
3	4	6	T2	T2	E	-9	286	5	4	6	E	T2	T1	32	5005
3	4	6	T2	T2	T1	-2	143	5	4	6	E	T2	AT2	-11	364
3	4	6	T2	T2	AT2	-55	2496	5	4	6	E	T2	BT2	81	1820
3	4	6	T2	T2	BT2	-27	832	5	4	6	AT1	T2	A2	5	208
3	4	7	A2	T2	AT1	7	715	5	4	6	BT1	T2	A2	-1	1456
3	4	7	A2	T2	BT1	-3	65	5	4	6	AT1	T2	E	25	2288
3	4	7	T1	T2	A2	1	33	5	4	6	BT1	T2	E	-77	1040
3	4	7	T1	T2	E	-1	39	5	4	6	AT1	T2	T1	3	2288
3	4	7	T1	T2	AT1	7	3432	5	4	6	BT1	T2	T1	-3	80080
3	4	7	T1	T2	BT1	-1	104	5	4	6	AT1	T2	AT2	5	18304

K= 4 ; HAMILTONIAN REP = T2							
J1	J2	J3	REP1	REP2	REP3	NUM**2	DEN**2
5	4	6	AT1	T2	BT2	9	1664
5	4	6	BT1	T2	AT2	-1156	512512
5	4	6	BT1	T2	BT2	-465	10412
5	4	6	T2	T2	A1	-5	572
5	4	6	T2	T2	E	-9	20020
5	4	6	T2	T2	T1	-125	4004
5	4	6	T2	T2	AT2	275	8736
5	4	6	T2	T2	BT2	-158	9467
5	4	7	E	T2	AT1	-358	8499
5	4	7	E	T2	BT1	-30	1547
5	4	7	E	T2	AT2	205	10634
5	4	7	E	T2	BT2	9	2380
5	4	7	AT1	T2	A2	-1	4488
5	4	7	BT1	T2	A2	265	12812
5	4	7	AT1	T2	E	1	5304
5	4	7	BT1	T2	E	-21	8840
5	4	7	AT1	T2	AT1	-124	6847
5	4	7	AT1	T2	BT1	-25	226304
5	4	7	BT1	T2	AT1	213	5962
5	4	7	BT1	T2	BT1	-153	465920
5	4	7	AT1	T2	AT2	-174	8513
5	4	7	AT1	T2	BT2	83	3007
5	4	7	BT1	T2	AT2	-37	1648
5	4	7	BT1	T2	BT2	-355	23736
5	4	7	T2	T2	E	-30	1547
5	4	7	T2	T2	AT1	2701	388942
5	4	7	T2	T2	BT1	206	15721
5	4	7	T2	T2	AT2	-164	10555
5	4	7	T2	T2	BT2	-45	182784
6	4	6	A1	T2	AT2	-1	155584
6	4	6	A1	T2	BT2	-196	6845
6	4	6	A2	T2	T1	-17	728
6	4	6	E	T2	T1	-185	13953
6	4	6	E	T2	AT2	232	8065
6	4	6	E	T2	BT2	28	6845
6	4	6	T1	T2	A2	17	728
6	4	6	T1	T2	E	185	13953
6	4	6	T1	T2	T1	136	12343
6	4	6	T1	T2	AT2	11	1547
6	4	6	T1	T2	BT2	45	1547
6	4	6	AT2	T2	A1	1	155584
6	4	6	BT2	T2	A1	196	6845
6	4	6	AT2	T2	E	-232	8065
6	4	6	BT2	T2	E	-28	6845
6	4	6	AT2	T2	T1	-11	1547
6	4	6	BT2	T2	T1	45	1547
6	4	6	AT2	T2	AT2	915	19922
6	4	6	AT2	T2	BT2	-54	396032
6	4	6	BT2	T2	AT2	54	396032
6	4	6	BT2	T2	BT2	-93	12401
6	4	7	A1	T2	AT2	152	4055
6	4	7	A1	T2	BT2	1	136
6	4	7	A2	T2	AT1	-9	17680
6	4	7	A2	T2	BT1	97	3893
6	4	7	E	T2	AT1	-18	77792
6	4	7	E	T2	BT1	-35	21479
6	4	7	E	T2	AT2	224	22275
6	4	7	E	T2	BT2	-1	952
6	4	7	T1	T2	A2	-75	2618
6	4	7	T1	T2	E	-3	3094
6	4	7	T1	T2	AT1	239	4173
6	4	7	T1	T2	BT1	177	13154
6	4	7	T1	T2	AT2	-51	26702
6	4	7	T1	T2	BT2	175	9791
6	4	7	AT2	T2	E	-158	13467
6	4	7	BT2	T2	E	-184	12421
6	4	7	AT2	T2	AT1	-299	9008
6	4	7	AT2	T2	BT1	4	25115
6	4	7	BT2	T2	AT1	-49	16200
6	4	7	BT2	T2	BT1	22	19781
6	4	7	AT2	T2	AT2	149	6620
6	4	7	AT2	T2	BT2	194	7707
6	4	7	BT2	T2	AT2	-109	13693
6	4	7	BT2	T2	BT2	175	16993
7	4	7	A2	T2	AT1	-191	14746

K= 4 ; HAMILTONIAN REP = T2							
J1	J2	J3	REP1	REP2	REP3	NUM**2	DEN**2
7	4	7	A2	T2	BT1	54	6259
7	4	7	E	T2	AT1	257	23449
7	4	7	E	T2	BT1	335	20654
7	4	7	E	T2	AT2	-75	235144
7	4	7	E	T2	BT2	568	23157
7	4	7	AT1	T2	A2	-191	14746
7	4	7	BT1	T2	A2	54	6259
7	4	7	AT1	T2	E	257	23449
7	4	7	BT1	T2	E	335	20654
7	4	7	AT1	T2	AT1	-35	4866
7	4	7	AT1	T2	BT1	18	1074944
7	4	7	BT1	T2	AT1	18	1074944
7	4	7	BT1	T2	BT1	123	28115
7	4	7	AT1	T2	AT2	-89	11693
7	4	7	AT1	T2	BT2	81	5168
7	4	7	BT1	T2	AT2	363	7694
7	4	7	BT1	T2	BT2	11	6783
7	4	7	AT2	T2	E	75	235144
7	4	7	BT2	T2	E	-568	23157
7	4	7	AT2	T2	AT1	-89	11693
7	4	7	AT2	T2	BT1	363	7694
7	4	7	BT2	T2	AT1	81	5168
7	4	7	BT2	T2	BT1	11	6783
7	4	7	AT2	T2	AT2	-317	2622738
7	4	7	AT2	T2	BT2	-19	182784
7	4	7	BT2	T2	AT2	-19	182784
7	4	7	BT2	T2	BT2	156	5197

K= 6 ; HAMILTONIAN REP = T2							
J1	J2	J3	REP1	REP2	REP3	NUM**2	DEN**2
0	6	6	A1	AT2	AT2	-3	13
0	6	6	A1	BT2	BT2	-3	13
1	6	5	T1	AT2	E	16	143
1	6	5	T1	AT2	AT1	105	18304
1	6	5	T1	AT2	BT1	178	2053
1	6	5	T1	BT2	BT1	-189	1664
1	6	5	T1	AT2	T2	-11	416
1	6	5	T1	BT2	T2	-45	416
1	6	6	T1	AT2	A2	11	728
1	6	6	T1	BT2	A2	-45	728
1	6	6	T1	AT2	E	5	728
1	6	6	T1	BT2	E	99	728
1	6	6	T1	AT2	T1	-375	2912
1	6	6	T1	BT2	T1	-33	2912
1	6	6	T1	AT2	AT2	119	2025
1	6	6	T1	AT2	BT2	431	20284
1	6	6	T1	BT2	AT2	-431	20284
1	6	6	T1	BT2	BT2	-9	23296
1	6	7	T1	AT2	A2	3	56
1	6	7	T1	BT2	A2	11	840
1	6	7	T1	AT2	E	-33	728
1	6	7	T1	BT2	E	13	840
1	6	7	T1	AT2	AT1	-3	832
1	6	7	T1	AT2	BT1	99	5824
1	6	7	T1	BT2	AT1	297	4160
1	6	7	T1	BT2	BT1	275	9522
1	6	7	T1	AT2	AT2	9	11648
1	6	7	T1	AT2	BT2	-99	896
1	6	7	T1	BT2	AT2	349	3493
1	6	7	T1	BT2	BT2	9	4480
2	6	4	E	AT2	T1	1	4290
2	6	4	E	BT2	T1	3	26
2	6	4	E	AT2	T2	-56	715
2	6	4	T2	AT2	A1	13	792
2	6	4	T2	BT2	A1	-5	104
2	6	4	T2	AT2	E	77	4680
2	6	4	T2	BT2	E	7	104
2	6	4	T2	AT2	T1	48	715
2	6	4	T2	AT2	T2	-112	2145
2	6	5	E	AT2	AT1	-12	143
2	6	5	E	AT2	BT1	27	5005
2	6	5	E	BT2	BT1	-3	91
2	6	5	E	AT2	T2	192	5005

K= 6 ; HAMILTONIAN REP = T2							K= 6 ; HAMILTONIAN REP = T2								
J1	J2	J3	REP1	REP2	REP3	NUM**2	DEN**2	J1	J2	J3	REP1	REP2	REP3	NUM**2	DEN**2
2	6	5	T2	AT2	E	27	5005	3	6	5	T2	AT2	BT1	166	9453
2	6	5	T2	BT2	E	-3	91	3	6	5	T2	BT2	AT1	45	832
2	6	5	T2	AT2	AT1	75	18304	3	6	5	T2	BT2	BT1	-9	5824
2	6	5	T2	AT2	BT1	-371	3985	3	6	5	T2	AT2	T2	-15	16016
2	6	5	T2	BT2	AT1	135	1664	3	6	5	T2	BT2	T2	-27	1456
2	6	5	T2	BT2	BT1	75	11648	3	6	6	A2	AT2	T1	243	8008
2	6	5	T2	AT2	T2	-81	160160	3	6	6	A2	BT2	T1	-15	728
2	6	5	T2	BT2	T2	-225	2912	3	6	6	T1	AT2	A2	21	832
2	6	6	E	AT2	T1	-27	1001	3	6	6	T1	BT2	A2	165	5824
2	6	6	E	BT2	T1	-3	455	3	6	6	T1	AT2	E	105	9152
2	6	6	E	AT2	AT2	30	1001	3	6	6	T1	BT2	E	-363	5824
2	6	6	E	BT2	BT2	-66	455	3	6	6	T1	AT2	T1	-45	4004
2	6	6	T2	AT2	A1	75	1144	3	6	6	T1	BT2	T1	-9	364
2	6	6	T2	BT2	A1	3	520	3	6	6	T1	AT2	AT2	-107	12659
2	6	6	T2	AT2	E	33	728	3	6	6	T1	AT2	BT2	135	11648
2	6	6	T2	BT2	E	-3	3640	3	6	6	T1	BT2	AT2	-135	11648
2	6	6	T2	AT2	T1	116	15291	3	6	6	T1	BT2	BT2	-33	11648
2	6	6	T2	BT2	T1	245	9827	3	6	6	T2	AT2	A1	147	9152
2	6	6	T2	AT2	AT2	-88	10227	3	6	6	T2	BT2	A1	-15	832
2	6	6	T2	AT2	BT2	329	7038	3	6	6	T2	AT2	E	-125	5046
2	6	6	T2	BT2	AT2	329	7038	3	6	6	T2	BT2	E	15	5824
2	6	6	T2	BT2	BT2	23	27061	3	6	6	T2	AT2	T1	631	14972
2	6	7	E	AT2	AT1	1	26	3	6	6	T2	BT2	T1	15	1456
2	6	7	E	AT2	BT1	-33	728	3	6	6	T2	AT2	BT2	-9	182
2	6	7	E	BT2	BT1	3	3640	3	6	6	T2	BT2	AT2	9	182
2	6	7	E	AT2	AT2	-9	364	3	6	7	A2	AT2	AT1	-125	2431
2	6	7	E	BT2	BT2	9	140	3	6	7	A2	AT2	BT1	-15	6188
2	6	7	T2	AT2	E	-33	728	3	6	7	A2	BT2	BT1	-33	6188
2	6	7	T2	BT2	E	3	3640	3	6	7	T1	AT2	A2	21	2992
2	6	7	T2	AT2	AT1	1	208	3	6	7	T1	BT2	A2	-332	8707
2	6	7	T2	BT2	AT1	33	1456	3	6	7	T1	AT2	E	-21	3536
2	6	7	T2	BT2	BT1	99	1040	3	6	7	T1	BT2	E	-361	8011
2	6	7	T2	BT2	BT1	3	7280	3	6	7	T1	AT2	AT1	157	13882
2	6	7	T2	AT2	AT2	21	1664	3	6	7	T1	AT2	BT1	-299	5608
2	6	7	T2	AT2	BT2	33	896	3	6	7	T1	BT2	AT1	70	11091
2	6	7	T2	BT2	AT2	-152	2217	3	6	7	T1	BT2	BT1	154	7079
2	6	7	T2	BT2	BT2	3	4480	3	6	7	T1	AT2	AT2	-1	26798
3	6	3	A2	AT2	T1	8	143	3	6	7	T1	AT2	BT2	143	26798
3	6	3	T1	AT2	A2	8	143	3	6	7	T1	BT2	AT2	159	9479
3	6	3	T1	AT2	T1	15	9152	3	6	7	T1	BT2	BT2	185	26948
3	6	3	T1	BT2	T1	75	832	3	6	7	T2	AT2	E	-15	6188
3	6	3	T1	AT2	T2	-13	704	3	6	7	T2	BT2	E	-33	6188
3	6	3	T1	BT2	T2	45	832	3	6	7	T2	AT2	AT1	115	18348
3	6	3	T2	AT2	T1	13	704	3	6	7	T2	AT2	BT1	252	5657
3	6	3	T2	BT2	T1	45	832	3	6	7	T2	BT2	AT1	-76	13225
3	6	3	T2	AT2	T2	352	4383	3	6	7	T2	BT2	BT1	-373	9624
3	6	3	T2	BT2	T2	-27	832	3	6	7	T2	AT2	AT2	321	10837
3	6	4	A2	AT2	T1	-10	3003	3	6	7	T2	AT2	BT2	-73	6571
3	6	4	A2	BT2	T1	6	91	3	6	7	T2	BT2	AT2	535	14311
3	6	4	T1	AT2	E	8	143	3	6	7	T2	BT2	BT2	231	69632
3	6	4	T1	AT2	T1	-125	9522	4	6	4	A1	AT2	T2	5	858
3	6	4	T1	BT2	T1	45	5824	4	6	4	A1	BT2	T2	1	78
3	6	4	T1	AT2	T2	307	7783	4	6	4	E	AT2	T1	-2	143
3	6	4	T1	BT2	T2	45	832	4	6	4	E	BT2	T1	-2	65
3	6	4	T2	AT2	A1	248	8447	4	6	4	E	AT2	T2	-7	858
3	6	4	T2	BT2	A1	5	182	4	6	4	E	BT2	T2	-7	390
3	6	4	T2	AT2	E	125	2574	4	6	4	T1	AT2	E	2	143
3	6	4	T2	BT2	E	-1	26	4	6	4	T1	BT2	E	2	65
3	6	4	T2	AT2	T1	290	15291	4	6	4	T1	AT2	T1	91	704
3	6	4	T2	BT2	T1	27	5824	4	6	4	T1	BT2	T1	7	4160
3	6	4	T2	AT2	T2	55	2496	4	6	4	T1	AT2	T2	11	832
3	6	4	T2	BT2	T2	27	832	4	6	4	T1	BT2	T2	49	4160
3	6	5	A2	AT2	AT1	-2	143	4	6	4	T2	AT2	A1	-5	858
3	6	5	A2	AT2	BT1	45	2002	4	6	4	T2	BT2	A1	-1	78
3	6	5	A2	BT2	BT1	9	182	4	6	4	T2	AT2	E	7	858
3	6	5	T1	AT2	E	8	1001	4	6	4	T2	BT2	E	7	390
3	6	5	T1	AT2	AT1	-338	8249	4	6	4	T2	AT2	T1	-11	832
3	6	5	T1	AT2	BT1	-33	5824	4	6	4	T2	BT2	T1	49	4160
3	6	5	T1	BT2	AT1	-3	832	4	6	4	T2	AT2	T2	175	9152
3	6	5	T1	BT2	BT1	-135	5824	4	6	4	T2	BT2	T2	343	4160
3	6	5	T1	AT2	T2	422	4937	4	6	5	A1	AT2	T2	-479	6826
3	6	5	T1	BT2	T2	-45	1456	4	6	5	A1	BT2	T2	1	208
3	6	5	T2	AT2	E	45	2002	4	6	5	E	AT2	AT1	-5	143
3	6	5	T2	BT2	E	9	182	4	6	5	E	AT2	BT1	-11	364
3	6	5	T2	AT2	AT1	-11	832	4	6	5	E	BT2	BT1	81	1820

K= 6 ; HAMILTONIAN REP = T2						K= 6 ; HAMILTONIAN REP = T2									
J1	J2	J3	REP1	REP2	REP3	NUM**2	DEN**2	J1	J2	J3	REP1	REP2	REP3	NUM**2	DEN**2
4	6	5	E	AT2	T2	-1	144144	4	6	7	T2	AT2	AT2	149	6620
4	6	5	E	BT2	T2	-7	1040	4	6	7	T2	AT2	BT2	194	7707
4	6	5	T1	AT2	E	-49	1716	4	6	7	T2	BT2	AT2	109	13693
4	6	5	T1	BT2	E	3	260	4	6	7	T2	BT2	BT2	-175	16993
4	6	5	T1	AT2	AT1	-35	18304	5	6	5	E	AT2	AT1	-10	2431
4	6	5	T1	AT2	BT1	1	18304	5	6	5	E	AT2	BT1	-63	4862
4	6	5	T1	BT2	AT1	63	1664	5	6	5	E	BT2	BT1	-63	2210
4	6	5	T1	BT2	BT1	-9	8320	5	6	5	E	AT2	T2	-63	4862
4	6	5	T1	AT2	T2	-3	4576	5	6	5	E	BT2	T2	-63	2210
4	6	5	T1	BT2	T2	27	2080	5	6	5	AT1	AT2	E	-10	2431
4	6	5	T2	AT2	E	11	364	5	6	5	BT1	AT2	E	-63	4862
4	6	5	T2	BT2	E	-81	1820	5	6	5	BT1	BT2	E	-63	2210
4	6	5	T2	AT2	AT1	5	18304	5	6	5	AT1	AT2	AT1	505	6633
4	6	5	T2	AT2	BT1	-1156	512512	5	6	5	AT1	AT2	BT1	-53	16627
4	6	5	T2	BT2	AT1	9	1664	5	6	5	AT1	BT2	AT1	-105	226304
4	6	5	T2	BT2	BT1	-465	10412	5	6	5	AT1	BT2	BT1	-456	13225
4	6	5	T2	AT2	T2	-275	8736	5	6	5	BT1	AT2	AT1	-53	16627
4	6	5	T2	BT2	T2	158	9467	5	6	5	BT1	AT2	BT1	-167	7611
4	6	6	A1	AT2	AT2	179	18001	5	6	5	BT1	BT2	AT1	-456	13225
4	6	6	A1	AT2	BT2	5	3536	5	6	5	BT1	BT2	BT1	462	22859
4	6	6	A1	BT2	AT2	5	3536	5	6	5	AT1	AT2	T2	-260	22411
4	6	6	A1	BT2	BT2	-99	3536	5	6	5	AT1	BT2	T2	-9	14144
4	6	6	E	AT2	T1	1058	272272	5	6	5	BT1	AT2	T2	-3087	155584
4	6	6	E	BT2	T1	181	5531	5	6	5	BT1	BT2	T2	63	70720
4	6	6	E	AT2	AT2	-10798	445416	5	6	5	T2	AT2	E	63	4862
4	6	6	E	AT2	BT2	-7	3536	5	6	5	T2	BT2	E	63	2210
4	6	6	E	BT2	AT2	-7	3536	5	6	5	T2	AT2	AT1	-260	22411
4	6	6	E	BT2	BT2	-246	12301	5	6	5	T2	AT2	BT1	-3087	155584
4	6	6	T1	AT2	A2	85	2496	5	6	5	T2	BT2	AT1	9	14144
4	6	6	T1	BT2	A2	33	14144	5	6	5	T2	BT2	BT1	-63	70720
4	6	6	T1	AT2	E	-71	24207	5	6	5	T2	AT2	T2	-97	28746
4	6	6	T1	BT2	E	-15	14144	5	6	5	T2	BT2	T2	139	5779
4	6	6	T1	AT2	T1	208	22411	5	6	6	E	AT2	T1	-27	4862
4	6	6	T1	BT2	T1	45	3536	5	6	6	E	BT2	T1	-15	442
4	6	6	T1	AT2	BT2	27	442	5	6	6	E	AT2	BT2	3	221
4	6	6	T1	BT2	AT2	27	442	5	6	6	E	BT2	AT2	-3	221
4	6	6	T2	AT2	A1	1	155584	5	6	6	AT1	AT2	A2	39	1904
4	6	6	T2	BT2	A1	196	6845	5	6	6	AT1	BT2	A2	-82	12301
4	6	6	T2	AT2	E	-232	8065	5	6	6	BT1	AT2	A2	-15	3536
4	6	6	T2	BT2	E	-28	6845	5	6	6	BT1	BT2	A2	33	3536
4	6	6	T2	AT2	T1	-11	1547	5	6	6	AT1	AT2	E	116	12459
4	6	6	T2	BT2	T1	-45	1547	5	6	6	AT1	BT2	E	315	21479
4	6	6	T2	AT2	AT2	-915	19922	5	6	6	BT1	AT2	E	33	3536
4	6	6	T2	AT2	BT2	54	396032	5	6	6	BT1	BT2	E	15	3536
4	6	6	T2	BT2	AT2	54	396032	5	6	6	AT1	AT2	T1	169	11330
4	6	6	T2	BT2	BT2	-93	12401	5	6	6	AT1	BT2	T1	-117	7616
4	6	7	A1	AT2	AT2	25	19448	5	6	6	BT1	AT2	T1	117	11968
4	6	7	A1	AT2	BT2	1	136	5	6	6	BT1	BT2	T1	45	14144
4	6	7	A1	BT2	AT2	5	15912	5	6	6	AT1	AT2	AT2	-83	1639
4	6	7	A1	BT2	BT2	55	1224	5	6	6	AT1	AT2	BT2	1604	1505742
4	6	7	E	AT2	AT1	-9	12155	5	6	6	AT1	BT2	AT2	-1604	1505742
4	6	7	E	AT2	BT1	-158	13467	5	6	6	AT1	BT2	BT2	-77	5400
4	6	7	E	BT2	BT1	-184	12421	5	6	6	BT1	AT2	AT2	101	10318
4	6	7	E	AT2	AT2	347	6341	5	6	6	BT1	AT2	BT2	5902	129254
4	6	7	E	AT2	BT2	-7	680	5	6	6	BT1	BT2	AT2	-5902	129254
4	6	7	E	BT2	AT2	-7	15912	5	6	6	BT1	BT2	BT2	75	22859
4	6	7	E	BT2	BT2	243	7571	5	6	6	T2	AT2	A1	-42	77792
4	6	7	T1	AT2	A2	-9	14960	5	6	6	T2	BT2	A1	-105	3536
4	6	7	T1	BT2	A2	1	2448	5	6	6	T2	AT2	E	51	2288
4	6	7	T1	AT2	E	-313	7591	5	6	6	T2	BT2	E	15	3536
4	6	7	T1	BT2	E	11	31824	5	6	6	T2	AT2	T1	1323	155584
4	6	7	T1	AT2	AT1	908	4429402	5	6	6	T2	BT2	T1	-283	10674
4	6	7	T1	AT2	BT1	70	11091	5	6	6	T2	AT2	BT2	9	1768
4	6	7	T1	BT2	AT1	431	6208	5	6	6	T2	BT2	AT2	-9	1768
4	6	7	T1	BT2	BT1	-95	6976	5	6	7	E	AT2	AT1	-83	3258
4	6	7	T1	AT2	AT2	-71	28593	5	6	7	E	AT2	BT1	-264	20275
4	6	7	T1	AT2	BT2	726	696320	5	6	7	E	BT2	BT1	131	5334
4	6	7	T1	BT2	AT2	113	7749	5	6	7	E	AT2	AT2	123	11831
4	6	7	T1	BT2	BT2	-6522	2643949	5	6	7	E	AT2	BT2	169	6460
4	6	7	T2	AT2	E	158	13467	5	6	7	E	BT2	AT2	-81	15796
4	6	7	T2	BT2	E	184	12421	5	6	7	AT1	AT2	A2	-54	1591744
4	6	7	T2	AT2	AT1	299	9008	5	6	7	AT1	BT2	A2	161	6418
4	6	7	T2	AT2	BT1	-4	25115	5	6	7	BT1	AT2	A2	-179	5256
4	6	7	T2	BT2	AT1	-49	16200	5	6	7	BT1	BT2	A2	27	19336
4	6	7	T2	BT2	BT1	22	19781	5	6	7	AT1	AT2	E	81	2821728

K= 6 ; HAMILTONIAN REP = T2							K= 6 ; HAMILTONIAN REP = T2								
J1	J2	J3	REP1	REP2	REP3	NUM**2	DEN**2	J1	J2	J3	REP1	REP2	REP3	NUM**2	DEN**2
5	6	7	AT1	BT2	E	167	5633	6	6	7	E	AT2	AT1	-650	227392
5	6	7	BT1	AT2	E	-63	25189	6	6	7	E	AT2	BT1	7623	403104
5	6	7	BT1	BT2	E	-891	403104	6	6	7	E	BT2	AT1	1089	671840
5	6	7	AT1	AT2	AT1	-1567	1531718	6	6	7	E	BT2	BT1	128	14891
5	6	7	AT1	AT2	BT1	-3581	1272806	6	6	7	E	AT2	AT2	-203	15655
5	6	7	AT1	BT2	AT1	379	1341246	6	6	7	E	AT2	BT2	7	5168
5	6	7	AT1	BT2	BT1	88	10115	6	6	7	E	BT2	AT2	31	18366
5	6	7	BT1	AT2	AT1	-124	26169	6	6	7	E	BT2	BT2	296	11037
5	6	7	BT1	AT2	BT1	-145	28453	6	6	7	T1	AT2	A2	-133	8976
5	6	7	BT1	BT2	AT1	-33	7031	6	6	7	T1	BT2	A2	-82	11211
5	6	7	BT1	BT2	BT1	113	5107	6	6	7	T1	AT2	E	175	201552
5	6	7	AT1	AT2	AT2	-50	13763	6	6	7	T1	BT2	E	-161	26014
5	6	7	AT1	AT2	BT2	136	14697	6	6	7	T1	AT2	AT1	-23	13951
5	6	7	AT1	BT2	AT2	36	18515	6	6	7	T1	AT2	BT1	91	41344
5	6	7	AT1	BT2	BT2	207	11458	6	6	7	T1	BT2	AT1	-39	206720
5	6	7	BT1	AT2	AT2	61	15216	6	6	7	T1	BT2	BT1	-96	14891
5	6	7	BT1	AT2	BT2	1513	5207364	6	6	7	T1	AT2	AT2	185	6888
5	6	7	BT1	BT2	AT2	109	6069	6	6	7	T1	AT2	BT2	261	25480
5	6	7	BT1	BT2	BT2	-7	5197	6	6	7	T1	BT2	AT2	157	10934
5	6	7	T2	AT2	E	264	20275	6	6	7	T1	BT2	BT2	-111	7358
5	6	7	T2	BT2	E	-131	5334	6	6	7	AT2	BT2	E	231	8398
5	6	7	T2	AT2	AT1	13	1333	6	6	7	BT2	AT2	E	-231	8398
5	6	7	T2	AT2	BT1	-251	9177242	6	6	7	AT2	AT2	AT1	427	8839
5	6	7	T2	BT2	AT1	567	1074943	6	6	7	AT2	AT2	BT1	315	806208
5	6	7	T2	BT2	BT1	125	4237	6	6	7	AT2	BT2	BT1	243	806208
5	6	7	T2	AT2	AT2	52	1249	6	6	7	AT2	BT2	BT1	693	806208
5	6	7	T2	AT2	BT2	-203	3528	6	6	7	BT2	AT2	AT1	-243	806208
5	6	7	T2	BT2	AT2	-45	19184	6	6	7	BT2	AT2	BT1	-693	806208
5	6	7	T2	BT2	BT2	-139	14216	6	6	7	BT2	BT2	AT1	-309	7928
6	6	6	A1	AT2	AT2	65	8331	6	6	7	BT2	BT2	BT1	364	21307
6	6	6	A1	AT2	BT2	-118	5393	6	6	7	AT2	BT2	AT2	-63	403104
6	6	6	A1	BT2	AT2	-33	33592	6	6	7	AT2	BT2	BT2	231	10336
6	6	6	A2	AT2	T1	-21	67184	6	6	7	BT2	AT2	AT2	-63	403104
6	6	6	A2	BT2	T1	131	7620	6	6	7	BT2	AT2	BT2	231	10336
6	6	6	E	AT2	T1	209	5090	7	6	7	A2	AT2	AT1	-75	14212
6	6	6	E	BT2	T1	-131	16764	7	6	7	A2	AT2	BT1	-7	1292
6	6	6	E	AT2	AT2	-148	9011	7	6	7	A2	BT2	AT1	-115	18419
6	6	6	E	AT2	BT2	92	29433	7	6	7	A2	BT2	BT1	-77	6460
6	6	6	E	BT2	AT2	92	29433	7	6	7	E	AT2	AT1	75	16796
6	6	6	E	BT2	BT2	-131	19050	7	6	7	E	AT2	BT1	77	16796
6	6	6	T1	AT2	A2	21	67184	7	6	7	E	BT2	AT1	-143	19380
6	6	6	T1	BT2	A2	-131	7620	7	6	7	E	BT2	BT1	847	83980
6	6	6	T1	AT2	E	-209	5090	7	6	7	E	AT2	AT2	42	4199
6	6	6	T1	BT2	E	131	16764	7	6	7	E	BT2	AT2	151	6862
6	6	6	T1	AT2	T1	-79	15130	7	6	7	AT1	AT2	A2	-75	14212
6	6	6	T1	BT2	T1	291	7345	7	6	7	AT1	BT2	A2	-115	18419
6	6	6	T1	AT2	BT2	-92	29433	7	6	7	BT1	AT2	A2	-7	1292
6	6	6	T1	BT2	AT2	-92	29433	7	6	7	BT1	BT2	A2	-77	6460
6	6	6	AT2	AT2	A1	-65	8331	7	6	7	AT1	AT2	E	75	16796
6	6	6	AT2	BT2	A1	118	5393	7	6	7	AT1	BT2	E	-143	19380
6	6	6	BT2	AT2	A1	118	5393	7	6	7	BT1	AT2	E	77	16796
6	6	6	BT2	BT2	A1	33	33592	7	6	7	BT1	BT2	E	847	83980
6	6	6	AT2	AT2	E	148	9011	7	6	7	AT1	AT2	AT1	-4532	166174
6	6	6	AT2	BT2	E	-92	29433	7	6	7	AT1	BT2	BT1	414	12991
6	6	6	BT2	AT2	E	-92	29433	7	6	7	AT1	BT2	AT1	318	11575270
6	6	6	BT2	BT2	E	131	19050	7	6	7	AT1	BT2	BT1	11	13005
6	6	6	AT2	BT2	T1	92	29433	7	6	7	BT1	AT2	AT1	414	12991
6	6	6	BT2	AT2	T1	92	29433	7	6	7	BT1	AT2	BT1	151	10179
6	6	6	AT2	AT2	AT2	38	13577	7	6	7	BT1	BT2	AT1	11	13005
6	6	6	AT2	AT2	BT2	-819	1323008	7	6	7	BT1	BT2	BT1	257	9408
6	6	6	AT2	BT2	AT2	-819	1323008	7	6	7	AT1	AT2	AT2	-152	26009
6	6	6	AT2	BT2	BT2	329	9663	7	6	7	AT1	AT2	BT2	-81	5292031
6	6	6	BT2	AT2	AT2	819	1323008	7	6	7	AT1	BT2	AT2	354	7793258
6	6	6	BT2	AT2	BT2	-329	9663	7	6	7	AT1	BT2	BT2	196	12399
6	6	6	BT2	BT2	AT2	-329	9663	7	6	7	BT1	AT2	AT2	1062	1449035
6	6	6	BT2	BT2	BT2	684	1543249	7	6	7	BT1	AT2	BT2	138	14651
6	6	7	A1	AT2	AT2	-186	13475	7	6	7	BT1	BT2	AT2	-68	29089
6	6	7	A1	AT2	BT2	-49	5168	7	6	7	BT1	BT2	BT2	-32	13329
6	6	7	A1	BT2	AT2	-195	16504	7	6	7	AT2	AT2	E	-42	4199
6	6	7	A1	BT2	BT2	98	25579	7	6	7	AT2	BT2	E	-151	6862
6	6	7	A2	AT2	AT1	-65	18336	7	6	7	AT2	AT2	AT1	152	26009
6	6	7	A2	AT2	BT1	-128	14891	7	6	7	AT2	AT2	BT1	-1062	1449035
6	6	7	A2	BT2	AT1	-297	403104	7	6	7	AT2	BT2	AT1	354	7793258
6	6	7	A2	BT2	BT1	7623	403104	7	6	7	AT2	BT2	BT1	-68	29089
6	6	7						7	6	7	BT2	AT2	AT1	81	5292031

K= 6			J HAMILTONIAN REP = T2				
J1	J2	J3	REP1	REP2	REP3	NUM**2	DEN**2
7	6	7	BT2	AT2	BT1	-138	14051
7	6	7	BT2	BT2	AT1	196	12399
7	6	7	BT2	BT2	BT1	-32	13329
7	6	7	AT2	AT2	AT2	111	19111
7	6	7	AT2	AT2	BT2	191	29629
7	6	7	AT2	BT2	AT2	1811	3797038
7	6	7	AT2	BT2	BT2	205	10462
7	6	7	BT2	AT2	AT2	191	29629

K=	J2	J3	HAMILTONIAN			REP = T1	DEN**2	K=	J2	J3	HAMILTONIAN			REP = T1	DEN**2
1	1	1	REP1	REP2	REP3	NUM**2	1	1	1	REP1	REP2	REP3	NUM**2	1	
1	1	1	A1	T1	T1	1	1	5	1	6	T2	T1	T1	15	572
1	1	1	T1	T1	T1	-1	1	5	1	6	T2	T1	AT2	11	416
1	1	2	T1	T1	E	2	5	5	1	6	T2	T1	BT2	-45	416
1	1	2	T1	T1	T2	3	5	6	1	6	A1	T1	T1	-1	13
1	1	2	E	T1	T2	-2	5	6	1	6	A2	T1	AT2	11	728
1	1	2	T2	T1	E	-2	5	6	1	6	A2	T1	BT2	-45	728
1	1	2	T2	T1	T2	1	5	6	1	6	E	T1	T1	-1	91
1	1	3	E	T1	T1	-9	35	6	1	6	E	T1	AT2	-5	728
1	1	3	E	T1	T2	1	7	6	1	6	E	T1	BT2	-99	728
1	1	3	T2	T1	A2	-1	7	6	1	6	T1	T1	A1	-1	13
1	1	3	T2	T1	T1	-6	35	6	1	6	T1	T1	E	-1	91
1	1	3	T2	T1	T2	2	7	6	1	6	T1	T1	T1	-1	364
1	1	3	A2	T1	T2	1	7	6	1	6	T1	T1	AT2	375	2912
1	1	3	T1	T1	T1	9	56	6	1	6	T1	T1	BT2	33	2912
1	1	3	T1	T1	T2	15	56	6	1	6	AT2	T1	A2	11	728
1	1	3	T2	T1	A2	-1	7	6	1	6	BT2	T1	A2	-45	728
1	1	3	T2	T1	T1	-15	56	6	1	6	AT2	T1	E	-5	728
1	1	3	T2	T1	T2	-1	56	6	1	6	BT2	T1	E	-99	728
1	1	4	A2	T1	T2	1	7	6	1	6	AT2	T1	T1	375	2912
1	1	4	T1	T1	A1	1	9	6	1	6	BT2	T1	T1	33	2912
1	1	4	T1	T1	E	-5	63	6	1	6	AT2	T1	AT2	119	2025
1	1	4	T1	T1	T2	5	168	6	1	6	AT2	T1	BT2	431	20284
1	1	4	T2	T1	E	1	7	6	1	6	BT2	T1	AT2	-431	20284
1	1	4	T2	T1	T1	-1	8	6	1	7	BT2	T1	BT2	-9	23296
1	1	4	T2	T1	T2	9	56	6	1	7	A1	T1	AT1	7	520
1	1	4	A1	T1	T1	-1	9	6	1	7	A1	T1	BT1	-33	520
1	1	4	E	T1	T1	-7	45	6	1	7	A2	T1	AT2	-99	1456
1	1	4	E	T1	T2	-1	15	6	1	7	A2	T1	BT2	1	112
1	1	4	T1	T1	A1	-1	9	6	1	7	E	T1	AT1	-49	520
1	1	4	T1	T1	E	-7	45	6	1	7	E	T1	BT1	-33	3640
1	1	4	T1	T1	T1	-1	120	6	1	7	E	T1	AT2	45	1456
1	1	4	T1	T1	T2	7	120	6	1	7	E	T1	BT2	11	560
1	1	4	T2	T1	E	-1	15	6	1	7	T1	T1	E	-33	455
1	1	4	T2	T1	T1	7	120	6	1	7	T1	T1	AT1	-9	520
1	1	4	T2	T1	T2	5	24	6	1	7	T1	T1	BT1	297	3640
1	1	5	A1	T1	AT1	-35	396	6	1	7	T1	T1	AT2	3	7280
1	1	5	A1	T1	BT1	-1	44	6	1	7	T1	T1	BT2	-33	560
1	1	5	E	T1	AT1	25	396	6	1	7	AT2	T1	A2	-3	56
1	1	5	E	T1	BT1	-7	220	6	1	7	BT2	T1	A2	-11	840
1	1	5	E	T1	T2	7	55	6	1	7	AT2	T1	E	-33	728
1	1	5	T1	T1	E	-3	55	6	1	7	BT2	T1	E	13	840
1	1	5	T1	T1	AT1	7	66	6	1	7	AT2	T1	AT1	-3	832
1	1	5	T1	T1	BT1	3	110	6	1	7	AT2	T1	BT1	99	5824
1	1	5	T1	T1	T2	8	55	6	1	7	BT2	T1	AT1	297	4160
1	1	5	T2	T1	E	7	55	6	1	7	BT2	T1	BT1	275	9522
1	1	5	T2	T1	AT1	-1	66	6	1	7	AT2	T1	AT2	-9	11648
1	1	5	T2	T1	BT1	21	110	6	1	7	AT2	T1	BT2	99	896
1	1	5	E	T1	BT1	-8	55	6	1	7	BT2	T1	AT2	-349	3493
1	1	5	E	T1	T2	-2	55	7	1	7	BT2	T1	BT2	-9	4480
1	1	5	BT1	T1	E	-8	55	7	1	7	A2	T1	AT2	13	1680
1	1	5	AT1	T1	AT1	-45	704	7	1	7	A2	T1	BT2	33	560
1	1	5	AT1	T1	BT1	-63	704	7	1	7	E	T1	BT1	-2	35
1	1	5	BT1	T1	AT1	-63	704	7	1	7	E	T1	AT2	11	1680
1	1	5	BT1	T1	BT1	11	320	7	1	7	E	T1	BT2	-39	560
1	1	5	AT1	T1	T2	21	176	7	1	7	BT1	T1	E	-2	35
1	1	5	BT1	T1	T2	-3	880	7	1	7	AT1	T1	AT1	35	1024
1	1	5	T2	T1	E	2	55	7	1	7	AT1	T1	BT1	297	5120
1	1	5	T2	T1	AT1	-21	176	7	1	7	BT1	T1	AT1	297	5120
1	1	5	T2	T1	BT1	3	880	7	1	7	BT1	T1	BT1	-133	2578
1	1	5	T2	T1	T2	-5	44	7	1	7	AT1	T1	AT2	135	2048
1	1	6	E	T1	T1	10	143	7	1	7	AT1	T1	BT2	406	9691
1	1	6	E	T1	AT2	-16	143	7	1	7	BT1	T1	AT2	199	10717
1	1	6	AT1	T1	A1	-9	572	7	1	7	BT1	T1	BT2	-97	6603
1	1	6	BT1	T1	A1	35	572	7	1	7	AT2	T1	A2	-13	1680
1	1	6	AT1	T1	E	63	572	7	1	7	BT2	T1	A2	-33	560
1	1	6	BT1	T1	E	5	572	7	1	7	AT2	T1	E	-11	1680
1	1	6	AT1	T1	T1	-63	2288	7	1	7	BT2	T1	E	39	560
1	1	6	BT1	T1	T1	245	2288	7	1	7	AT2	T1	AT1	-135	2048
1	1	6	AT1	T1	AT2	105	18304	7	1	7	AT2	T1	BT1	-199	10717
1	1	6	BT1	T1	BT2	-189	1664	7	1	7	BT2	T1	AT1	-486	9691
1	1	6	BT1	T1	AT2	178	2053	7	1	7	BT2	T1	BT1	97	6603
1	1	6	BT1	T1	BT2	-15	1664	7	1	7	AT2	T1	AT2	-494	5355
1	1	6	T2	T1	A2	-1	13	7	1	7	AT2	T1	BT2	87	9691
1	1	6	T2	T1	E	5	143	7	1	7	BT2	T1	AT2	87	9691
1	1	6	T2	T1	E	5	143	7	1	7	BT2	T1	BT2	-69	11762

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41. Ref. [6], Eq. (2.18)
42. Ref. [5], Table A11