Spectroscopic Coefficients for the p^n, d^n, and f^n Configurations

C. W. Nielson and George F. Koster

Spectroscopic Coefficients for the p^n, d^n, and f^n Configurations

C. W. Nielson and George F. Koster

The M.I.T. Press
Massachusetts Institute of Technology
Cambridge, Massachusetts

Library of Congress Catalog Card Number: 63-23154
Printed in the United States of America

PREFACE

This book consists of a set of tables useful for theoretical studies of atoms and ions in p^n, d^n, and f^n configurations. In a series of papers appearing between 1942 and 1949, Racah systematized the analysis of the energy levels of atoms and introduced methods that supplemented the earlier work of Slater so useful for the analysis of the energy levels of the lighter atoms. Using Racah's methods, one can find closed expressions for the matrix elements of operators with known transformation properties and for the matrices determining the energy levels of ions in the ℓ^n configurations. Involved in these expressions, there occur quantities that, if tabulated, greatly facilitate the evaluation of matrix elements. Of these the Clebsch-Gordan coefficients (or the related 3-j symbols), Racah W coefficients (or the related 6-j symbols), and the coefficients of fractional parentage play a central role. The first two of these three sets of coefficients are already well tabulated. There is the recent excellent tabulation by Manuel Rotenberg, R. Bivins, N. Metropolis, and John K. Wooten, Jr. in their book The 3-j and 6-j Symbols (Technology Press, Cambridge, Mass., 1959). The coefficients of fractional parentage, which relate the states of an ℓ^n configuration to those of an ℓ^{n-1} (its "parent"), are not tabulated as thoroughly. They exist in Racah's papers for p^n and d^n configurations and are analyzed for the f^n configurations in these papers. This set of tables contains the coefficients of fractional parentage for f^n configurations.

In addition to these three sets of coefficients, there are algebraic combinations of them that occur with sufficient frequency to warrant tabulation. These occur in the calculation of matrix elements of tensor operators and are the so-called "reduced matrix elements." Some of the more useful of these are also included in this tabulation.

The authors wish to express their appreciation for fruitful discussions with Dr. P. Nutter, Dr. A. Runciman, Dr. A. D. Pierce, Prof. J. C. Slater, and members of the Solid State and Molecular Theory Group at M. I. T. The computations were done at the M. I. T. Cooperative Computing Laboratory and were supported by the Office of Naval Research and the National Science Foundation.

Cambridge, Massachusetts
October, 1963

C. W. Nielson
George F. Koster

INTRODUCTION

Many problems of atomic structure with applications in chemical and solid-state physics can be most efficiently solved by means of the tensor-operator methods originated by Racah. Several descriptions of these methods have been published recently.[1-5] In order to use the methods, certain mathematical quantities are required, notably reduced matrix elements for standard configurations and 3-j and 6-j symbols. Rather comprehensive coverage of 3-j and 6-j symbols is given in the tabulation by Rotenberg et. al.[6] The present book presents reduced matrix elements and related quantities for all possible configurations of equivalent p, d, and f electrons. Part of the material is a recalculation of results already available in the literature,[4,7-12] but most of the results on f electrons are new. This introduction contains only sufficient information to identify accurately the contents of the tables. For information concerning the use and significance of these quantities, the reader is referred to the previously mentioned books.

Classification of States

Throughout this work, atomic states are considered to be constructed by L-S coupling. This coupling scheme is convenient for the tensor-operator methods and is conventionally used. Because more than one multiplet of a given L, S may occur, some further differentiation of the multiplets is required. For this purpose we have followed consistently the classification scheme of Racah[8] wherein additional quantum numbers, usually not of physical significance, are introduced by reference to the properties of certain mathematical groups. Specifically, the groups used are those denoted by R_5 in the case of the configurations d^n and by R_7 and G_2 for the configurations f^n. The so-called seniority quantum number is consistent with this scheme. Even with these additional quantum numbers, some duplications occur for f^n configurations, which were resolved arbitrarily by Racah in his work on the electrostatic energy of f^n configurations.[8]

The present tabulations are totally consistent with all of these choices, although the special quantum numbers themselves are actually printed only once. To identify matrix elements more compactly, a label is given to each multiplet, consisting of the multiplicity followed by the letter representation of the orbital angular momentum. When more than one multiplet of a particular multiplicity and orbital angular momentum occur, each is assigned a final sequential index. The exact correspondence between this label and the Racah quantum numbers is given in the listing of states at the beginning of the tables. The configurations p^n do not require any extra quantum numbers. The listings of d^n states give the label, the seniority number, and the R_5 representation symbol, in that order. The listings of f^n states give the label, the seniority, the R_7 representation symbol, and finally the G_2 representation symbol. Thereafter, only the label, comprising multiplicity, orbital angular momentum, and perhaps a sequential index, is used in the tables. For most applications, the explicit Racah quantum numbers are not required.

Fractional Parentage Coefficients

Fractional parentage coefficients were introduced by Racah[7] to facilitate computation of matrix elements for complicated configurations. They are important because all antisymmetric states of n electrons can be expressed as linear combinations of the states obtained by angular-momentum coupling one additional electron to the antisymmetric states of n-1 electrons. The coefficients of these linear combinations are the fractional parentage coefficients.

Racah has shown that fractional parentage coefficients can be factored if the states to which they refer correspond to his special group theoretical classification scheme; he calculated many of the factors needed for f^n configurations.[8] These factors and all others needed were newly computed[13] and assembled to give the complete set of fractional parentage coefficients in this book. In the tabulation, the first column specifies the final state, while the second gives the parent state. The fractional parentage coefficient connecting the two follows in powers-of-primes form. Zero coefficients are omitted completely from this section.

Electrostatic Matrix Elements

The electrostatic interaction energy for a configuration ℓ^n is usually specified in terms of the Slater F^k integrals[14] and is so specified here for the configurations p^n and d^n. For configurations f^n, Racah[8] introduced linear combinations of the F^k integrals which prove to be convenient and which are used in the present tabulation:

$$E^0 = F^0 - 2F^2/45 - F^4/33 - 50F^6/1287$$

$$E^1 = 14F^2/405 + 7F^4/297 + 350F^6/11583$$

$$E^2 = F^2/2025 - F^4/3267 + 175F^6/1656369$$

$$E^3 = F^2/135 + 2F^4/1089 - 175F^6/42471$$

Since the matrix is symmetric, only the upper diagonal half is given. Elements not diagonal in L and S are zero and are omitted from the tables.

These electrostatic matrix elements were calculated in a recursive manner starting with those of the ℓ^2 configuration and operating on them with a formula derived by Racah[15] until the maximum configurations were reached. In this way the electrostatic energy matrix is assured of referring to states with the same phase conventions as the fractional parentage coefficients and other quantities calculated from them. In actual practice, this correspondence was sometimes used in reverse to specify the phase of new fractional parentage coefficients so as to give ultimate agreement with previously published electrostatic matrix elements.

Reduced Matrix Elements

The exact definition for reduced matrix element used here is such that the actual matrix element

$$(L, M|T^K_Q|L', M')$$

of the tensor operator T^K_Q between initial state L, M and final state L', M' and the corresponding reduced matrix element $(L\|T^K\|L')$ are related by the equation

$$(L, M|T^K_Q|L', M') = (-1)^{L-M}\begin{pmatrix} L & K & L' \\ -M & Q & M' \end{pmatrix}(L\|T^K\|L')$$

where

$$\begin{pmatrix} L & K & L' \\ -M & Q & M' \end{pmatrix}$$

is the Wigner 3-j symbol. Racah introduced unit tensor operators[16] in terms of which other tensor operators may be expressed, and the reduced matrix elements for the unit tensor operators U^2, U^3, U^4, U^5, U^6, and V^{11} are tabulated here for the configurations p^n, d^n, and f^n. The reduced matrix element of a tensor operator is zero unless a triangle can be formed with the three angular momenta L, K, and L', and cases not fulfilling this condition are not listed at all. However, all other zeros are listed explicitly. Only the upper diagonal half of a matrix is given; the reflected elements are found from the equations

$$(\alpha' S' L'\|U^K\|\alpha SL) = (-1)^{L'-L}(\alpha SL\|U^K\|\alpha' S' L')$$

$$(\alpha' S' L'\|V^{1K}\|\alpha SL) = (-1)^{L'-L+S'-S} \times (\alpha LS\|V^{1K}\|\alpha' S' L')$$

All of these reduced matrix elements were calculated from fractional parentage coefficients and 6-j symbols using a formula from Racah.[17] This procedure assures complete consistency among the fractional parentage coefficients, electrostatic matrix elements, and the reduced matrix elements.[18]

Almost Closed Shells

With each state of ℓ^n there is associated a state of $\ell^{4\ell+2-n}$ that has the same quantum numbers.[16,19] Simple relationships exist between these two configurations, called conjugate configurations.

If the fractional parentage coefficient relating the $\alpha'S'L'$ state of ℓ^{n+1} to the αSL state of ℓ^n is denoted by

$$F(\ell^{n+1}\alpha'S'L';\ \ell^n\alpha SL)$$

then

$$F(\ell^{4\ell+2-n}\alpha SL;\ \ell^{4\ell+1-n}\alpha'S'L')$$

$$= \zeta(-1)^{S+S'+L+L'-\ell-\frac{1}{2}}\left[\frac{(n+1)(2S'+1)(2L'+1)}{(4\ell+2-n)(2S+1)(2L+1)}\right]^{\frac{1}{2}}$$

$$\times F(\ell^{n+1}\alpha'S'L';\ \ell^n\alpha SL)$$

where ζ is unity unless $n = 2\ell$. For $n = 2\ell$, $\zeta = (-1)^{\nu'-\frac{1}{2}}$, where ν' is the seniority number associated with $\alpha'S'L'$. The various sign factors are ultimately arbitrary, but they are not independent of other sign conventions that have already been assumed and must therefore be used.[20]

The electrostatic energy matrices for conjugate configurations are identical except for the addition of a constant diagonal term.[19]

The unit tensor operator reduced matrix elements for conjugate states are the same up to a sign factor:[7]

$$(\alpha SL\|U^K(4\ell+2-n)\|\alpha'S'L') = -(-1)^K(\alpha SL\|U^K(n)\|\alpha'S'L')$$

$$(\alpha SL\|V^{1K}(4\ell+2-n)\|\alpha'S'L') = (-1)^K(\alpha SL\|V^{1K}(n)\|\alpha'S'L')$$

Number Representation

Fractional parentage coefficients and reduced matrix elements are presented in a powers-of-primes representation consisting of twelve signed integers:

$$a_0 \quad a_1\ a_2\ a_3\ a_4 \quad a_5\ a_6\ a_7\ a_8 \quad a_9\ a_{10}\ a_{11}$$

These integers represent the real number

$$a_0\left(\prod_{i=1}^{11} p_i^{a_i}\right)^{\frac{1}{2}}$$

where p_i is the i^{th} prime. The first eleven primes are 2, 3, 5, 7, 11, 13, 17, 19, 23, 29, 31. In order to limit the powers to one printed column, the letters A, B, C, · · · are used to denote the rarely occuring powers 10, 11, 12, · · · . Zeros to the right in the array are omitted. As an example,

-37 -2 1 -1

represents the quantity

$$-\frac{37}{10}(15)^{\frac{1}{2}}$$

Electrostatic energy matrix elements are not given in powers-of-primes form because each such element comprises several terms, and it is convenient to use a notation sufficiently compact to present all terms on one line. To this end, something like ordinary algebraic notation is used, with the convention that the square root of a number is indicated by enclosing the number in parentheses. Thus

-72(429)E3/11

represents

$$-\frac{72}{11}(429)^{\frac{1}{2}}\ E^3$$

Programming Procedures

In order to reduce the possibility of error to a minimum, the tables were generated in an almost completely automatic manner with a digital computer. The powers-of-primes method was used in the computer itself for all computations. Coded lists of the states corresponding to each configuration were prepared by hand. Computer programs, using these lists as a guide, then generated all quantities here tabulated. A supervisory program concurrently composed the results into page form, adding headings and page numbering. When a page was completed, it was written onto magnetic tape. The entire book was prepared twice in this way, and the tapes compared, thus eliminating random errors from the results. Finally one of the tapes was printed on a line printer equipped with both tape checking and print-wheel checking devices. The printer output was then photographically reproduced.

REFERENCES

1. E. P. Wigner, Group Theory, Academic Press Inc., New York (1959).
2. A. R. Edmonds, Angular Momentum in Quantum Mechanics, Princeton University Press, Princeton, N. J. (1957).
3. U. Fano and G. Racah, Irreducible Tensorial Sets, Academic Press Inc., New York (1959).
4. J. C. Slater, Quantum Theory of Atomic Structure, Vol. II, McGraw-Hill Book Company, Inc., New York (1960). The appendices of this book contain extensive tabulations of coefficients for many configurations of s, p, and d electrons.
5. B. R. Judd, Operator Techniques in Atomic Spectroscopy, McGraw-Hill Book Company, Inc., New York (1963).
6. M. Rotenberg, R. Bivens, N. Metropolis, and J. K. Wooten, Jr., The 3-j and 6-j Symbols, Technology Press, Cambridge, Mass. (1959).
7. G. Racah, Phys. Rev., 63, 367 (1943).
8. G. Racah, Phys. Rev., 76, 1352 (1949).
9. B. R. Judd, Proc. Roy. Soc., A250, 565 (1959).
10. B. R. Judd and R. Loudon, Proc. Roy. Soc., A251, 127 (1959).
11. M. H. Crozier and W. A. Runciman, J. Chem. Phys., 35, 1392.
12. B. G. Wybourne, J. Chem. Phys., 36, 2301 (1962).
13. C. W. Nielson, Ph.D. Thesis, Department of Physics, M.I.T. (1962), unpublished.
14. J. C. Slater, Phys. Rev., 34, 1293 (1929).
15. Reference 8, Equation (1).
16. G. Racah, Phys. Rev., 62, 438 (1942).
17. Reference 7, Equation (23).
18. It should be noted that some of the results of Reference 12 do not agree with the present work. This occurs because of a lack of consistency between the factors reported in Reference 12 and the electrostatic matrix elements of Reference 8. The present tables are consistent and follow the conventions for factors implicit in Reference 8.
19. E. U. Condon and G. H. Shortley, The Theory of Atomic Spectra, Chaps. XII and XIII, Cambridge University Press, Cambridge. Reprinted with corrections (1951).
20. Reference 7, Equations (19) and (65).

CONTENTS

STATES OF P1

2P			

STATES OF P2

3P		1S		1D	

STATES OF P3

4S		2P		2D	

STATES OF D1

2D	1 (10)

STATES OF D2

3P	2 (11)	1S	0 (00)	1G	2 (20)
3F	2 (11)	1D	2 (20)		

STATES OF D3

4P	3 (11)	2P	3 (21)	2D2	3 (21)	2G	3 (21)
4F	3 (11)	2D1	1 (10)	2F	3 (21)	2H	3 (21)

STATES OF D4

5D	4 (10)	3F1	2 (11)	1S1	0 (00)	1F	4 (22)
3P1	2 (11)	3F2	4 (21)	1S2	4 (22)	1G1	2 (20)
3P2	4 (21)	3G	4 (21)	1D1	2 (20)	1G2	4 (22)
3D	4 (21)	3H	4 (21)	1D2	4 (22)	1I	4 (22)

STATES OF D5

6S	5 (00)	4G	5 (20[illegible]	2D2	[illegible] (2[illegible])	2G1	3 (21)
4P	3 (11)	2S	5 (2[illegible])	2D3	3 (22)	2G2	5 (22)
4D	5 (20)	2P	3 (2[illegible])	2F1	3 (21)	2H	3 (21)
4F	3 (11)	2D1	1 (1[illegible])	2F2	5 (22)	2I	5 (22)

STATES OF F1

2F	1 (100) (10)

STATES OF F2

3P	2 (110) (11)	3H	2 (110) (11)	1D	2 (200) (20)	1I	2 (200) (20)
3F	2 (110) (10)	1S	0 (000) (00)	1G	2 (200) (20)		

STATES OF F3

4S	3 (111) (00)	2P	3 (210) (11)	2G1	3 (210) (20)	2K	3 (210) (21)
4D	3 (111) (20)	2D1	3 (210) (20)	2G2	3 (210) (21)	2L	3 (210) (21)
4F	3 (111) (10)	2D2	3 (210) (21)	2H1	3 (210) (11)		
4G	3 (111) (20)	2F1	1 (100) (10)	2H2	3 (210) (21)		
4I	3 (111) (20)	2F2	3 (210) (21)	2I	3 (210) (20)		

STATES OF F4

5S	4 (111) (00)	3F3	4 (211) (21)	3K2	4 (211) (30)	1G3	4 (220) (21)
5D	4 (111) (20)	3F4	4 (211) (30)	3L	4 (211) (21)	1G4	4 (220) (22)
5F	4 (111) (10)	3G1	4 (211) (20)	3M	4 (211) (30)	1H1	4 (220) (21)
5G	4 (111) (20)	3G2	4 (211) (21)	1S1	0 (000) (00)	1H2	4 (220) (22)
5I	4 (111) (20)	3G3	4 (211) (30)	1S2	4 (220) (22)	1I1	2 (200) (20)
3P1	2 (110) (11)	3H1	2 (110) (11)	1D1	2 (200) (20)	1I2	4 (220) (20)
3P2	4 (211) (11)	3H2	4 (211) (11)	1D2	4 (220) (20)	1I3	4 (220) (22)
3P3	4 (211) (30)	3H3	4 (211) (21)	1D3	4 (220) (21)	1K	4 (220) (21)
3D1	4 (211) (20)	3H4	4 (211) (30)	1D4	4 (220) (22)	1L1	4 (220) (21)
3D2	4 (211) (21)	3I1	4 (211) (20)	1F	4 (220) (21)	1L2	4 (220) (22)
3F1	2 (110) (10)	3I2	4 (211) (30)	1G1	2 (200) (20)	1N	4 (220) (22)
3F2	4 (211) (10)	3K1	4 (211) (21)	1G2	4 (220) (20)		

STATES OF F5

6P	5 (110) (11)	4H3	5 (211) (30)	2F3	5 (221) (10)	2I2	5 (221) (20)
6F	5 (110) (10)	4I1	3 (111) (20)	2F4	5 (221) (21)	2I3	5 (221) (30)
6H	5 (110) (11)	4I2	5 (211) (20)	2F5	5 (221) (30)	2I4	5 (221) (31)A
4S	3 (111) (00)	4I3	5 (211) (30)	2F6	5 (221) (31)A	2I5	5 (221) (31)B
4P1	5 (211) (11)	4K1	5 (211) (21)	2F7	5 (221) (31)B	2K1	3 (210) (21)
4P2	5 (211) (30)	4K2	5 (211) (30)	2G1	3 (210) (20)	2K2	5 (221) (21)
4D1	3 (111) (20)	4L	5 (211) (21)	2G2	3 (210) (21)	2K3	5 (221) (30)
4D2	5 (211) (20)	4M	5 (211) (30)	2G3	5 (221) (20)	2K4	5 (221) (31)A
4D3	5 (211) (21)	2P1	3 (210) (11)	2G4	5 (221) (21)	2K5	5 (221) (31)B
4F1	3 (111) (10)	2P2	5 (221) (11)	2G5	5 (221) (30)	2L1	3 (210) (21)
4F2	5 (211) (10)	2P3	5 (221) (30)	2G6	5 (221) (31)	2L2	5 (221) (21)
4F3	5 (211) (21)	2P4	5 (221) (31)	2H1	3 (210) (11)	2L3	5 (221) (31)
4F4	5 (211) (30)	2D1	3 (210) (20)	2H2	3 (210) (21)	2M1	5 (221) (30)
4G1	3 (111) (20)	2D2	3 (210) (21)	2H3	5 (221) (11)	2M2	5 (221) (31)
4G2	5 (211) (20)	2D3	5 (221) (20)	2H4	5 (221) (21)	2N	5 (221) (31)
4G3	5 (211) (21)	2D4	5 (221) (21)	2H5	5 (221) (30)	2O	5 (221) (31)
4G4	5 (211) (30)	2D5	5 (221) (31)	2H6	5 (221) (31)A		
4H1	5 (211) (11)	2F1	1 (100) (10)	2H7	5 (221) (31)B		
4H2	5 (211) (21)	2F2	3 (210) (21)	2I1	3 (210) (20)		

7F	6	(100)	(10)
5S	4	(111)	(00)
5P	6	(210)	(11)
5D1	4	(111)	(20)
5D2	6	(210)	(20)
5D3	6	(210)	(21)
5F1	4	(111)	(10)
5F2	6	(210)	(21)
5G1	4	(111)	(20)
5G2	6	(210)	(20)
5G3	6	(210)	(21)
5H1	6	(210)	(11)
5H2	6	(210)	(21)
5I1	4	(111)	(20)
5I2	6	(210)	(20)
5K	6	(210)	(21)
5L	6	(210)	(21)
3P1	2	(110)	(11)
3P2	4	(211)	(11)
3P3	4	(211)	(30)
3P4	6	(221)	(11)
3P5	6	(221)	(30)
3P6	6	(221)	(31)
3D1	4	(211)	(20)
3D2	4	(211)	(21)
3D3	6	(221)	(20)
3D4	6	(221)	(21)
3D5	6	(221)	(31)
3F1	2	(110)	(10)
3F2	4	(211)	(10)
3F3	4	(211)	(21)
3F4	4	(211)	(30)
3F5	6	(221)	(10)
3F6	6	(221)	(21)
3F7	6	(221)	(30)
3F8	6	(221)	(31)A
3F9	6	(221)	(31)B
3G1	4	(211)	(20)
3G2	4	(211)	(21)
3G3	4	(211)	(30)
3G4	6	(221)	(20)
3G5	6	(221)	(21)
3G6	6	(221)	(30)
3G7	6	(221)	(31)
3H1	2	(110)	(11)
3H2	4	(211)	(11)
3H3	4	(211)	(21)
3H4	4	(211)	(30)
3H5	6	(221)	(11)
3H6	6	(221)	(21)
3H7	6	(221)	(30)
3H8	6	(221)	(31)A
3H9	6	(221)	(31)B
3I1	4	(211)	(20)
3I2	4	(211)	(30)
3I3	6	(221)	(20)
3I4	6	(221)	(30)
3I5	6	(221)	(31)A
3I6	6	(221)	(31)B
3K1	4	(211)	(21)
3K2	4	(211)	(30)
3K3	6	(221)	(21)
3K4	6	(221)	(30)
3K5	6	(221)	(31)A
3K6	6	(221)	(31)B
3L1	4	(211)	(21)
3L2	6	(221)	(21)
3L3	6	(221)	(31)
3M1	4	(211)	(30)
3M2	6	(221)	(30)
3M3	6	(221)	(31)
3N	6	(221)	(31)
3O	6	(221)	(31)
1S1	0	(000)	(00)
1S2	4	(220)	(22)
1S3	6	(222)	(00)
1S4	6	(222)	(40)
1P	6	(222)	(30)
1D1	2	(200)	(20)
1D2	4	(220)	(20)
1D3	4	(220)	(21)
1D4	4	(220)	(22)
1D5	6	(222)	(20)
1D6	6	(222)	(40)
1F1	4	(220)	(21)
1F2	6	(222)	(10)
1F3	6	(222)	(30)
1F4	6	(222)	(40)
1G1	2	(200)	(20)
1G2	4	(220)	(20)
1G3	4	(220)	(21)
1G4	4	(220)	(22)
1G5	6	(222)	(20)
1G6	6	(222)	(30)
1G7	6	(222)	(40)A
1G8	6	(222)	(40)B
1H1	4	(220)	(21)
1H2	4	(220)	(22)
1H3	6	(222)	(30)
1H4	6	(222)	(40)
1I1	2	(200)	(20)
1I2	4	(220)	(20)
1I3	4	(220)	(22)
1I4	6	(222)	(20)
1I5	6	(222)	(30)
1I6	6	(222)	(40)A
1I7	6	(222)	(40)B
1K1	4	(220)	(21)
1K2	6	(222)	(30)
1K3	6	(222)	(40)
1L1	4	(220)	(21)
1L2	4	(220)	(22)
1L3	6	(222)	(40)A
1L4	6	(222)	(40)B
1M1	6	(222)	(30)
1M2	6	(222)	(40)
1N1	4	(220)	(22)
1N2	6	(222)	(40)
1Q	6	(222)	(40)

STATES OF F7

8S	7	(000)	(00)
6P	5	(110)	(11)
6D	7	(200)	(20)
6F	5	(110)	(10)
6G	7	(200)	(20)
6H	5	(110)	(11)
6I	7	(200)	(20)
4S1	3	(111)	(00)
4S2	7	(220)	(22)
4P1	5	(211)	(11)
4P2	5	(211)	(30)
4D1	3	(111)	(20)
4D2	5	(211)	(20)
4D3	5	(211)	(21)
4D4	7	(220)	(20)
4D5	7	(220)	(21)
4D6	7	(220)	(22)
4F1	3	(111)	(10)
4F2	5	(211)	(10)
4F3	5	(211)	(21)
4F4	5	(211)	(30)
4F5	7	(220)	(21)
4G1	3	(111)	(20)
4G2	5	(211)	(20)
4G3	5	(211)	(21)
4G4	5	(211)	(30)
4G5	7	(220)	(20)
4G6	7	(220)	(21)
4G7	7	(220)	(22)
4H1	5	(211)	(11)
4H2	5	(211)	(21)
4H3	5	(211)	(30)
4H4	7	(220)	(21)
4H5	7	(220)	(22)
4I1	3	(111)	(20)
4I2	5	(211)	(20)
4I3	5	(211)	(30)
4I4	7	(220)	(20)
4I5	7	(220)	(22)
4K1	5	(211)	(21)
4K2	5	(211)	(30)
4K3	7	(220)	(21)
4L1	5	(211)	(21)
4L2	7	(220)	(21)
4L3	7	(220)	(22)
4M	5	(211)	(30)
4N	7	(220)	(22)
2S1	7	(222)	(00)
2S2	7	(222)	(40)
2P1	3	(210)	(11)
2P2	5	(221)	(11)
2P3	5	(221)	(30)
2P4	5	(221)	(31)
2P5	7	(222)	(30)
2D1	3	(210)	(20)
2D2	3	(210)	(21)
2D3	5	(221)	(20)
2D4	5	(221)	(21)
2D5	5	(221)	(31)
2D6	7	(222)	(20)
2D7	7	(222)	(40)
2F1	1	(100)	(10)
2F2	3	(210)	(21)
2F3	5	(221)	(10)
2F4	5	(221)	(21)
2F5	5	(221)	(30)
2F6	5	(221)	(31)A
2F7	5	(221)	(31)B
2F8	7	(222)	(10)
2F9	7	(222)	(30)
2F10	7	(222)	(40)
2G1	3	(210)	(20)
2G2	3	(210)	(21)
2G3	5	(221)	(20)
2G4	5	(221)	(21)
2G5	5	(221)	(30)
2G6	5	(221)	(31)
2G7	7	(222)	(20)
2G8	7	(222)	(30)
2G9	7	(222)	(40)A
2G10	7	(222)	(40)B
2H1	3	(210)	(11)
2H2	3	(210)	(21)
2H3	5	(221)	(11)
2H4	5	(221)	(21)
2H5	5	(221)	(30)
2H6	5	(221)	(31)A
2H7	5	(221)	(31)B
2H8	7	(222)	(30)
2H9	7	(222)	(40)
2I1	3	(210)	(20)
2I2	5	(221)	(20)
2I3	5	(221)	(30)
2I4	5	(221)	(31)A
2I5	5	(221)	(31)B
2I6	7	(222)	(20)
2I7	7	(222)	(30)
2I8	7	(222)	(40)A
2I9	7	(222)	(40)B
2K1	3	(210)	(21)
2K2	5	(221)	(21)
2K3	5	(221)	(30)
2K4	5	(221)	(31)A
2K5	5	(221)	(31)B
2K6	7	(222)	(30)
2K7	7	(222)	(40)
2L1	3	(210)	(21)
2L2	5	(221)	(21)
2L3	5	(221)	(31)
2L4	7	(222)	(40)A
2L5	7	(222)	(40)B
2M1	5	(221)	(30)
2M2	5	(221)	(31)
2M3	7	(222)	(30)
2M4	7	(222)	(40)
2N1	5	(221)	(31)
2N2	7	(222)	(40)
2O	5	(221)	(31)
2Q	7	(222)	(40)

FRACTIONAL PARENTAGE P2

```
3P    2P      1
1S    2P      1
1D    2P      1
```

FRACTIONAL PARENTAGE P3

```
4S    3P      1
2P    3P     -1    -1
      1S      1     1-2
      1D     -1    -1-2 1
2D    3P      1    -1
      1D     -1    -1
```

FRACTIONAL PARENTAGE D2

```
3P    2D      1
3F    2D      1
1S    2D      1
1D    2D      1
1G    2D      1
```

FRACTIONAL PARENTAGE D3

```
4P    3P     -1     3-1-1
      3F     -1     0-1-1 1
4F    3P     -1     0 0-1
      3F      1     2 0-1
2P    3P      1    -1-1-1 1
      3F     -1     2-1-1
      1D      1    -1
2D1   3P     -1    -2 1-1
      3F     -1    -2 0-1 1
      1S      1     2-1-1
      1D     -1    -2-1
      1G     -1    -2 1-1
2D2   3P     -1    -2 0-1 1
      3F      1    -2 1-1
      1D      1    -2 2 0-1
      1G     -1    -2 0 1-1
2F    3P      1     1 0-1
      3F      1    -1 0-1
      1D     -1     0 0 0-1
      1G     -1    -1 0 1-1
2G    3F      1    -1
      1D     -1     0-1 1-1
      1G      1    -1-1 0-1    1
2H    3F     -1    -1
      1G      1    -1
```

FRACTIONAL PARENTAGE D4

```
5D    4P      1    -1 1-1
      4F      1    -1 0-1 1
3P1   4P     -1     3-2-1
      4F     -1     0-2-1 1
      2P     -1    -2-2-1 1
      2D1     1    -3 1
      2D2    -1    -3-2 0 1
      2F     -1     0-2-1 1
3P2   4P     -1     0-2-1 1
      4F      1     3-2-1
      2P      1    -1-2 1
      2D2     1     0-2
      2F     -1    -1-2 1
3D    4P      1    -1-1-1 1
      4F     -1    -1 0-1
      2P     -1     0-1-1
      2D2     1     1 0 0-1
      2F     -1    -1 0-1
      2G      1    -1 1 0-1
3F1   4P     -1     0-1-1
      4F      1     2-1-1
      2P      1     1-1-1-1
      2D1     1    -3 1
      2D2     1    -3 0 0-1
      2F     -1    -2-1-1
      2G      1    -2 1 0-1
      2H      1    -2-1 0-1    1
3F2   4P     -1     2-1-1
      4F     -1     0-1-1
      2P     -1    -1-1 1-1
      2D2     1    -1 0 0-1
      2F     -1    -4-1 1
      2G     -1    -4 3 0-1
      2H      1    -2-1 0-1    1
3G    4F     -1     0-1
      2D2     1    -1-1 1-1
      2F      1    -4 1
      2G      1    -4 2-1-1    1
      2H      1    -2-1-1 0    1
3H    4F      1     0-1
      2F      1    -2-1
      2G     -1    -2 1-1
      2H      1    -1-1-1 0    0 1
```

FRACTIONAL PARENTAGE D4

1S1	2D1	1		
1S2	2D2	1		
1D1	2P	-1	-2 1-1	
	2D1	1	-3 1	
	2D2	1	-3 2 0-1	
	2F	1	-1 0-1	
	2G	-1	-1 1 0-1	
1D2	2P	1	-1 1-1	
	2D2	1	0 0 0-1	
	2F	1	-2 2-1	
	2G	1	-2 1 0-1	
1F	2P	1	-1 1 0-1	
	2D2	1	-1 0 1-1	
	2F	-1	-4 1	
	2G	-1	-4 1-1-1	
	2H	-1	-2 1-1-1	1
1G1	2D1	1	-3 1	
	2D2	-1	-3-2 2-1	
	2F	1	-2-2 1	
	2G	1	-2-1 0-1	1
	2H	-1	-2-2 0 0	1
1G2	2D2	1	-1-2 0-1	1
	2F	1	-4-2 1 0	1
	2G	-1	-4-1 0-1	0 2
	2H	-1	-2-2	
1I	2G	1	-1 1-1	
	2H	1	-1 0-1 1	

FRACTIONAL PARENTAGE D5

6S	5D	1		
4P	5D	-1	-2	
	3P1	-1	4-1-2	
	3P2	1	-1-1-2 1	
	3D	1	-2-1-1 1	
	3F1	-1	1-1-2 1	
	3F2	1	1-1-2 1	
4D	5D	-1	-2	
	3P2	1	-1 2-2	
	3D	-1	-2 3-1-1	
	3F2	-1	0 1-2	
	3G	1	0 2-1-1	
4F	5D	-1	-2	
	3P1	-1	1 0-2	
	3P2	-1	2 0-2-1	
	3D	-1	-2 1-1-1	
	3F1	1	3 0-2	
	3F2	1	-1 0-2	
	3G	-1	-1 2-1-1	
	3H	-1	-1 0-1-1	1
4G	5D	-1	-2	
	3D	1	-2-1 1-1	
	3F2	-1	-1-1	
	3G	-1	-1 0-1-1	1
	3H	1	-1-1-1 0	1
2S	3D	1	0 1-1	
	1D2	-1	1 0-1	
2P	3P1	1	0-1-2 1	
	3P2	1	-1-1	
	3D	1	0-1-1	
	3F1	-1	3-1-2	
	3F2	-1	-1-1	
	1D1	1	0 0-1	
	1D2	1	-1 0-1	
	1F	-1	-1 0-1	
2D1	3P1	-1	-1 2-2	
	3F1	-1	-1 1-2 1	
	1S1	1	0 1-2	
	1D1	-1	-1 0-1	
	1G1	-1	-1 2-2	
2D2	3P1	-1	-1 0-2 1	
	3P2	-1	0 0-2	
	3D	1	1 1-1-1	
	3F1	1	-1 1-2	
	3F2	-1	-1 1-2	
	3G	1	-1 2-1-1	
	1S2	-1	0 0-2	
	1D1	1	-1 2-1-1	
	1D2	-1	0 0-1-1	
	1F	1	-1 0-1	
	1G1	-1	-1 0 0-1	
	1G2	-1	-1 0-2-1	1
2D3	3P2	1	-1 2-2	
	3D	1	0 1-1-1	
	3F2	1	-2 3-2	
	3G	1	-2 2-1-1	
	1S2	-1	1 0-2	
	1D2	1	-1 2-1-1	
	1F	1	-2 0-1	
	1G2	1	-2 2-2-1	1
2F1	3P1	1	2 0-2	
	3P2	-1	-1 0 0-1	
	3D	1	-1 1-1-1	
	3F1	1	0 0-2	
	3F2	-1	-4	
	3G	-1	-4 4-1-1	
	3H	1	-2 0-1-1	1
	1D1	-1	1 0-1-1	
	1D2	1	-2 2-1-1	
	1F	1	-4 1-1	
	1G1	-1	0 0 0-1	
	1G2	1	-4 0 0-1	1
2F2	3P2	1	-1 2-1-1	
	3D	1	-1 1 0-1	
	3F2	-1	-4 2-1	
	3G	-1	-4 2-2-1	
	3H	-1	-2 2-2-1	1
	1D2	-1	-2 0 0-1	
	1F	-1	-4 1	
	1G2	1	-4 2-1-1	1
2G1	3D	1	-1 0 0-1	
	3F1	1	0 0-1	
	3F2	1	-4 2-1	
	3G	1	-4 3-2-1	1
	3H	1	-2 0-2 0	1
	1D1	-1	1-1 0-1	
	1D2	-1	-2-1 0-1	
	1F	-1	-4-1-2	
	1G1	1	0-1-1-1	1
	1G2	1	-4-1-1-1	0 2
	1I	-1	-1-1-2 0	0 1
2G2	3D	1	-1-1-1-1	1
	3F2	1	-4-1 0 0	1
	3G	-1	-4 0-1-1	0 2
	3H	-1	-2-1-1	
	1D2	1	-2 0-1-1	1
	1F	-1	-4 0-1 0	1
	1G2	-1	-4 4 0-1	-1
	1I	-1	-1 0-1 0	-1 1
2H	3F1	-1	0 0-1	
	3F2	1	-2 0-1	
	3G	-1	-2 2-2	
	3H	1	-1 0-2 0	0 1
	1F	1	-2 1-2	
	1G1	1	0 0-1	
	1G2	-1	-2 0-1 0	-1
	1I	1	-1 0-2 1	-1 1
2I	3G	1	-1 2-2	
	3H	1	-1 1-2 1	
	1G2	-1	-1 2-1 0	-1
	1I	-1	-1 0 0 1	-1