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EMPIRICAL METHODS FOR CALCULATION OF BOND ENERGIES

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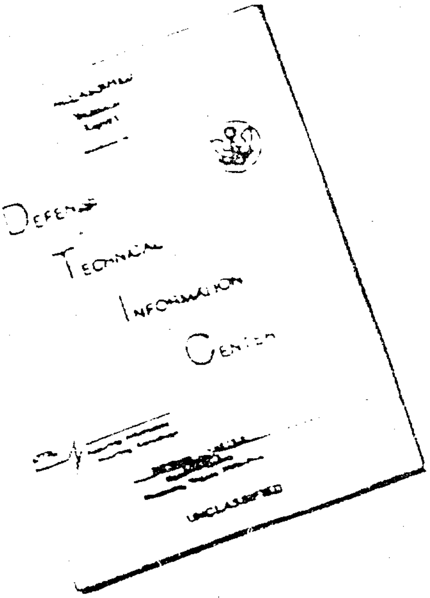
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FOREWORD

This report was prepared by the University of Cincinnati under USAF Contract No. AF 33(616)-6900. This contract was initiated Project No. 7023, "Research on Chemical Synthesis", Task No. 73666, "New Synthetic Methods for Polymers and Fluids." The work was administered under the direction of the Materials Central, Deputy for Advanced Systems Technology, Aeronautical Systems Division, with Lt. Robert J. McHenry acting as project engineer.

This report covers work conducted from January 1960 to January 1961.

ABSTRACT

Slater parameters (F's and G's) were calculated for the elements scandium to bromine and are tabulated. These parameters were used to calculate the energies of a wide variety of valence states of these elements, and of their unipositive ions, and hence valence state ionization potentials are derived. These data are tabulated.

PUBLICATION REVIEW

This report has been reviewed and is approved.

FOR THE COMMANDER

A. M. Lovelace

A. M. LOVELACE
Chief, Polymer Branch
Nonmetallic Materials Laboratory
Materials Central

TABLE OF CONTENTS

LIST OF TABLES

LIST OF TABLES (Continued)

LIST OF TABLES (continued)

I. INTRODUCTION

The present work, aimed at developing semi-empirical methods for estimating bond energies, is a continuation of work initiated by Jaffé and Doak (1). This work was based on an approximate application of Mulliken's "Magic Formula (2) to estimate carbon-metal bond energies in symmetrical metal alkyls.

The "Magic Formula" is an empirical equation, based on a combination of the essential features of both molecular orbital and valence bond theory, expressing the atomization energy of a compound in terms of a series of terms which can either be estimated theoretically or semiempirically. It has the form

$$D_o = \sum X_{ij} - \tfrac{1}{2}\sum Y_{kl} + \tfrac{1}{2}\sum K_{mn} - PE + RE$$

where the X_{ij} term is the energy resulting from the interaction of bonding electrons and is assumed to be expressed as

$$X_{ij} = A\, S_{ij}\, \bar{I}_{ij}/(1 + S_{ij})$$

A is an empirical coefficient, adjusted by Mulliken from work on some selected compounds of first row elements, and has a value of 1.16. The $\bar{I}_{ij}$ are the mean valence state ionization potentials of atoms i and j, and the S_{ij} are overlap integrals.

The Y_{kl} and K_{mn} are electron repulsion energies, which have been neglected in the present work, but the importance of which is now under investigation.

The promotion energy, PE, is defined as the energy required to promote the atoms to their respective valence states. The resonance energy, RE, is intended to account for all resonance terms of the valence bond theory, not included in the other terms.

In the original work (1), a long series of approximations were made. Y_{kl} and K_{mn} terms were neglected. In the evaluation of X_{ij}, normal ionization potentials were used instead of valence state ionization potentials. Only a single hybridization was considered, and promotion energies were neglected. Resonance energies were assumed to involve only ionic resonance energies, and were evaluated from electronegativities of the atoms.

Goldfarb (3) has started an investigation aimed at a removal of some of these drastic assumptions. The present work is intended to continue this process. The most important step which needs to be taken

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is the calculation of the required promotion energies and valence state ionization potentials for a variety of possible hybrid states of the atoms of concern. Later, investigation of the Y_{kl} and K_{mn} and of the electronegativities is planned.

The calculation of the needed valence state ionization potentials and promotion energies is based on calculation of the energies of valence states. Two methods are available for such calculations. One, due to Mulliken (4), is based on Slater's treatment of the complex atom (5). It involves expression of the valence state energy in terms of certain integrals over the radial atomic wave functions $F^k_{l,l}$ and $G^k_{l,l}$, the so-called Slater parameters. The other, proposed by Moffitt (6), expands the energy of valence states directly in terms of energies of spectroscopic (stationary) states of the atom. If the Slater treatment of the complex atom involved no assumptions, and hence no approximations, the two methods would be equivalent. Unfortunately, however, considerable approximations are involved in the Slater method; the worst of these are probably the neglect of configuration interaction and of spin-orbit coupling, and the assumption of perfect Russell-Saunders coupling. We believe that the Mulliken method, by averaging over more states, tends to minimize these approximations. Also, this method appears to lend itself more readily to machine calculation, and hence we have chosen this method. Consequently Slater parameters were needed for all elements of interest. The present report summarizes the parameters obtained, and the valence state promotion energies and ionization potentials computed with their aid.

II. METHODS AND RESULTS

A. Slater Equations for Stationary States.-The Slater parameters may be computed theoretically from the atomic radial wave functions. Such computations, however, are time-consuming. They would either involve finding, in the literature, the wave functions of all the atoms and ions needed, almost necessarily obtained in the same or equivalent approximation, or their calculation. No such data appear to be available in an approximation better than Slater orbitals, which was deemed inadequate for the present purpose. Although a Hartree-Fock calculation could undoubtedly be programmed, it was not deemed desirable to spend the time required to do so and carry out the massive computation involved.

Consequently, a semi-empirical technique was employed which is based on the well-known energies of spectroscopic states (7). In order to make use of these data, expressions for the energies of the spectroscopic states were required. These were obtained using a program written in this laboratory for the IBM 650 MDDPM (3). Since the methods are well-known, no details will be given.

B. Slater Parameters.-Given the equations for the energies of spectroscopic states in terms of the Slater parameters and empirical energy values, it should be a simple matter to solve for the parameters. However, a number of problems arise.

In the transition elements, generally a large number of spectroscopic states are observed and consequently more equations are available than parameters which need to be evaluated. Since the theory on which the equations are based is approximate, different values would be obtained by different choice of equations. The most logical procedure to follow under these circumstances appears a least squares method, which gives the values of the parameters which best represent all data. Accordingly, the equations were fitted by a standard multiple regression technique, using the IBM 650 MDDPM to carry out the needed computation.

Theory does not require the Slater parameters to be identical for different configurations, since the radial wave-functions generally differ. However, quite frequently, insufficient experimental data are available to find all parameters involved in a single configuration from the states of that configuration alone. Further, the equation for hybrid valence states of a given configuration frequently involves parameters not available from any states of the same configuration. Thus, e.g. in the valence state of carbon involving four tetrahedral hybrids, $(sp^3)^4$ or t_e^4, F_{ss} terms are required which do not enter into any of the spectroscopic states of the same configuration sp^3 of carbon. Accordingly, it was assumed throughout that the parameters could be treated as constants for an element, independent of the configuration, and multiple regression was generally performed on data from all configurations of interest, pooled into one regression. Calculations for single configurations are also reported, and tend to indicate that the overall fit of the equations was not appreciably adversely affected by this procedure, so that it may be concluded that the approximation involved in the assumption of constants F's and G's is less serious than some of the other approximations.

In cases where the number of equations was equal to the number of data, the parameters could, of course, be calculated directly by solution of the simultaneous equations, and this was done. In a few cases, some of the parameters could not be obtained at all, either because of lack of experimental data, or because of the nature of the equations. In such cases the missing parameters were estimated by extrapolation methods, or from theoretical calculations in the literature.

The experimental energies of spectroscopic states were taken from the tabulations of Moore (7). In states of higher multiplicity than one, means were used, weighted according to (2j+1). Where several states of equal L and S (equivalent multiplets) occur in the same configuration, the sum of all of them was used, since the Slater equation program was unable to perform the configuration interaction calculation needed to seperate the states.

Each energy expression involves, aside from the Slater parameters, a term constant for each configuration, W^o. The W^o for the lowest (ground state) configuration is treated as the constant term (intercept) of the multiple regression. The W^o terms of the other configurations were treated as a sum, W^o of the lowest configuration, and ΔW^o, the excess above this. The ΔW^o's were treated as additional parameters in the multiple regression.

The input data for the multiple regression analysis are given in Tables 1-24. In these tables, the first column specifies the configuration, the second the spectroscopic state, the last its energy, and the intervening columns give the energy equation. The results of the multiple regressions are shown in Tables 25-49. The first row gives the degrees of freedom available in the analysis, the second F, the variance ratio, and subsequent rows give the W_o's, F's and G's. Where available, standard deviations are given. Estimated values are so indicated.

The terms $F_2(dd)$ and $F_4(dd)$ of CuI are calculated by extrapolation of the corresponding parameters of FeI, CoI, and NiI. Values computed for CoI agree well with theoretically calculated ones (8). None of the $F_2(pp)$ terms for Fe, Co, Ni or Cu can be calculated from spectroscopic data. In accord with general practice, they have been neglected throughout.

In the calculation of valence state energies, some W^o values for higher configurations are often needed which cannot be calculated from empirical data. Such values have been estimated on the basis of the assumption that promotion of an electron from an x orbital to a y orbital requires the same energy for any configuration, so that the promotion xy ⟶ yy requires the same energy as xx ⟶ xy. Hence,

$$W_o(xy) - W_o(xx) = W_o(yy) - W_o(xy)$$

$$W_o(xx) - 2W_o(xy) + W_o(yy) = 0$$

so that the unknown parameter $W_o(yy)$ is estimated as

$$W_o(yy) = 2W_o(xy) - W_o(xx)$$

There are frequently different possible ways of making such estimates, which permit the testing of the assumption. Thus, $W_o(d^6p^2)$ of FeI, which is unobtainable empirically since no states of this configuration have been observed, may be estimated by any of the following three independent ways:

$$W_o(d^6p^2) = 2W_o(d^7p) - W_o(d^8) = 82,572.73 \text{ cm}^{-1}$$

$$W_o(d^6p^2) = W_o(d^7p) - W_o(d^6sp) - W_o(d^7s) = 103,155.52 \text{ cm}^{-1}$$

$$W_o(d^6p^2) = 2W_o(d^6sp) - W_o(d^6s^2) = 104,899.66 \text{ cm}^{-1}$$

Two of these are seen to agree excellently, the third only moderately well. Similarly for $W_o(d^5p^2)$ of FeII:

$$\begin{aligned} W_o(d^5p^2) &= 2W_o(d^6p) - W_o(d^7) = 178,598.39 \text{ cm}^{-1} \\ &= W_o(d^6p) + W_o(d^5sp) - W_o(d^6s) = 198,020.38 + G'_{sp} \text{ cm}^{-1} \\ &= 2W_o(d^5sp) - W_o(d^5s^2) = 193,668.22 + G'_{sp} \text{ cm}^{-1} \end{aligned}$$

suggesting $W_o(d^5p^2) = 178,598.39 \text{ cm}^{-1}$ and $G'_{sp} = 17,000 \text{ cm}^{-1}$. This type of relation was required repeatedly, and is referred to as the Δ_o relation.

C. Valence State Equations.-A valence state is defined as the state of an atom in which it exists in the molecule. Such states are not stationary states, and hence not observable, but are purely hypothetical states which can, however, be treated theoretically.

The formation of a valence state may be conceived as follows: Remove all atoms, with their electrons, from a central atom in a molecule, holding at the same time the electrons of the central atom fixed, i.e. at constant angular momentum and spin. In this process there results the valence state, in which the orbital angular momentum of each electron is fixed, while the spin is completely unknown. This lack of knowledge of spin arises because, in the molecule, each electron is paired with an electron from another atom, and removal of these other electrons leaves the electrons of the central atom with indeterminate spin.

The energy of such valence states can be treated exactly analogously to the energy of spectroscopic states (4). A program was written which permitted the generation of the energy of the valence states in terms of the Slater parameters discussed above. This program requires specification of a configuration, including information as to which electrons are to be considered as valence electrons, and of the wave function of any electrons occupying hybrid orbitals. It is capable of handling any configuration made up of any number of s, p and d electrons. In case the electrons not involved in bonding (non-bonding electrons) do not completely fill the available orbitals, the program makes computations for all possible assignments of d electrons to d orbitals and p electrons to p orbitals (9).

This program has been used to derive the energy equations, in terms of the Slater parameters, for a wide variety of valence states of the elements scandium through bromine. The valence states were specified in terms of the hybrid orbitals involved in the bonds. No complete treatment of all possible hybrids is possible, but it is believed that a sufficient variety of configurations and hybrids was included to permit the recognition of trends. The hybrids chosen were those believed, for each configuration, to be the ones most likely to lead to the formation of stable bonds. For each element, the most commonly observed coordination numbers were chosen, and in addition higher coordination numbers (four) were included. The hybrid orbitals used are summarized in Table 50, where σ, π, π', δ, δ' refers to the five d orbitals, d_{z^2}, d_{xz}, d_{yz}, d_{xy} and $d_{x^2-y^2}$, respectively, and x, y and z refers to the orbitals p_x, p_y and p_z, respectively.

The valence state ionization potential is defined as the energy required to remove an electron from one of the bonding orbitals of the atom in its valence state. Thus, the energy is required of the rather peculiar valence state of the ion with the one valence electron of the free atom missing. The program just described is capable of deriving the equations for such valence states, and was used to obtain the valence states for the ions.

D. Valence State Energies.-Given the valence state equations (cf. Section II C) and the Slater parameters (Section IIB), it is a simple matter of substitution to obtain valence state energies. The only difficulty that arises is that the valence state equation specifies the energy in terms of all the Slater parameters, including $F^o_{1,1'}$ and $G^o_{1,1'}$, whereas these quantities, since they occur equally in every spectroscopic state of a given configuration, cannot be evaluated empirically, but are included in the W^o terms. However, in a valence state of a given configuration, they occur in a different manner. Thus, since each of the orbitals of the $(sp^3)^4$ (te^4) state of carbon, e.g., involves a contribution from the s orbital, F^o_{ss} appears in the valence state equation, together with F^o_{sp} and F^o_{pp}. In the spectroscopic states of sp^3 carbon, however, only one electron is in the s orbital, and hence F^o_{ss} does not occur. Consequently it is necessary to eliminate the F^o's before the substitution can be performed. This is always possible by taking an appropriate combination of W^o's, three, $W^o(p^n)$, $W^o(p^{n-1}s)$, and $W^o(p^{n-2}s^2)$, in the case of s and p electrons only, and six $W^o(d^n)$, $W^o(d^{n-1}s)$, $W^od^{n-1}p$, $W^od^{n-2}s^2$, $W^o(d^{n-2}sp)$, and $W^o(d^{n-2}p^2)$ in the case of s,p, and d electrons. Also, in the case of more than half-filled shells, the spectroscopic states are calculated on the basis of complementary configurations, i.e. configurations in which vacancies are treated like electrons,

electrons like vacancies. This treatment also requires adjustment of W^o's. These eliminations, adjustments, and the subsequent substitution are not difficult. However, since the calculations were desired for several hundred valence states, a program for the IBM 650 MDDPM was written to perform all these functions. This program uses as input the output from the valence state equation program, and the data from the multiple regression, i.e. the Slater parameters, and finally produces the valence state energies.

It was not felt necessary to calculate the valence state ionization potentials for all possible valence states of any given configuration and hybrid type. Among the many possible states of a given configuration the one with the lowest promotion energy was chosen. This was invariably one of highest multiplicity, in accord with Hund's rule. Within a given multiplicity, energy differences were, in general, quite small, and it is believed that no significant differences exist. Calculations for the ion were then restricted to the particular valence state chosen, and results are given only for these states. These results are shown in Tables 51-60.

Finally, valence state ionization potentials are calculated by adding the normal ionization potential, obtained from Moore's tables (8) and the promotion energy of the ion, and subtracting the promotion energy of the atom.

III. DISCUSSION

The data presented in the accompanying Tables should prove useful for many calculations. In particular, they will be used for substitution into the Mulliken magic formula, both in the X_{ij} terms and as promotion energies PE. In addition, they will be used, when supplemented by electron affinities now being computed, in the calculation of electronegativities for elements in various hybrid states. In addition, calculation of Y_{kl} and K_{mn} integrals, now under investigation, will provide all terms needed for an application of the magic formula.

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Table 1. Multiple regression analysis input data for Sc I.

Conf.	Multp.	(d^2p)	ΔW_o (d^3)	(dsp)	(dp^2)	$F_2(pd)$	$F_2(dd)$	$F_4(dd)$	$G_1(pd)$	$G_3(pd)$	G_1sp	G_2sd	W cm^{-1}
d^2s	4F	0	0	0	0	0	-8	-9	0	0	0	-2	11,591.00
	2F	0	0	0	0	0	-8	-9	0	0	0	1	14,984,11
	2D	0	0	0	0	0	-3	36	0	0	0	-1	17,018.90
	4P	0	0	0	0	0	7	-84	0	0	0	-2	17,955.69
	^2G	0	0	0	0	0	4	1	0	0	0	-1	20,238.49
	^2P	0	0	0	0	0	7	-84	0	0	0	1	21,440.00
d^2p	^4G	1	0	0	0	11	-8	-9	-9	-12	0	0	29,152.50
	^2P	1	0	0	0	4	18	78	2	-24	0	0	30,639.10
	^4F	1	0	0	0	-3	-8	-9	-1	-48	0	0	31,253.00
	^4D(2/2)	1	0	0	0	0.5	-0.5	-48.5	-2	-58.5	0	0	38,642.27
	^2G(2/2)	1	0	0	0	-5	-2	-4	6	,-6	0	0	36,255.62
	^2D(3/3)	1	0	0	0	1.33	-1.33	-19	0	10	0	0	37,948.20
	^2F(3/3)	1	0	0	0	2.	-3.5	14	-1.5	-19.5	0	0	36,550.00
	^4S	1	0	0	0	-14	7	-84	6	-42	0	0	38,179.92
	^4P	1	0	0	0	7	7	-84	-6	-63	0	0	38,601.50
	^2H	1	0	0	0	4	4	1	-6	-3	0	0	39,199.42
	^2S	1	0	0	0	-14	7	-83	-3	21	0	0	43,287.00
d^3	^4F	0	1	0	0	0	-15	-72	0	0	0	0	33,828.25
	^2D	0	1	0	0	0	10	6	0	0	0	0	36,303.76
	^4P	0	1	0	0	0	0	-47	0	0	0	0	36,526.33
spd	^4F	0	0	1	0	2	0	0	-6	-3	-1	-1	15,881.76
	^4D	0	0	1	0	-7	0	0	3	-21	-1	-1	16,141.04
	^2D(2/2)	0	0	1	0	-3.5	0	0	0	0	0	0	20,499.98
	^4P	0	0	1	0	7	0	0	-1	-63	-1	-1	18,535.77
dp^2	^4F	0	0	0	1	-2	0	0	-6	-18	0	0	46,543.00
	^2D	0	0	0	1	1.33	0	0	066	-8	0	0	51,280.50

Table 2. Multiple regression analysis input data for Sc II

Config.	Multp.	ΔW_o					F_2pd	F_2dd	F_4dd	G_1pd	G_3pd	G_1sp	G_2sd	W
		(sd)	(p^2)	(d^2)	(sp)	(pd)								
s^2	^1S	0	0	0	0	0	0	0	0	0	0	0	0	11,736.35
ds	^3D	1	0	0	0	0	0	0	0	0	0	0	1	111.37
	^1D	1	0	0	0	0	0	0	0	0	0	0	-1	2,540.97
p^2	^3P	0	1	0	0	0	0	0	0	0	0	0	0	76,396.90
d^2	^3F	0	0	1	0	0	0	-8	-9	0	0	0	0	4,890.67
	^1D	0	0	1	0	0	0	-3	36	0	0	0	0	10,944.51
	^1G	0	0	1	0	0	0	4	1	0	0	0	0	14,261.40
	^3P	0	0	1	0	0	0	7	-84	0	0	0	0	12,109.67
sp	^3P	0	0	0	1	0	0	0	0	0	0	-1	0	39,153.65
	^1P	0	0	0	1	0	0	0	0	0	0	1	0	55,715.52
pd	^1D	0	0	0	0	1	-7	0	0	-3	21	0	0	26,081.32
	^3F	0	0	0	0	1	2	0	0	-6	-3	0	0	27,628.67
	^3D	0	0	0	0	1	-7	0	0	3	-21	0	0	28,039.21
	^3P	0	0	0	0	1	7	0	0	-1	-63	0	0	29,767.00
	^1P	0	0	0	0	1	7	0	0	1	63	0	0	30,815.65
	^1F	0	0	0	0	1	2	0	0	6	3	0	0	32,349.98

Table 3. Multiple regression analysis input data for Ti I.

Conf.	Multp.	ΔW_o (d^3s)	(d^3p)	(d^2sp)	(d^4)	(d^2p^2)	F_2pp	F_2pd	F_2dd	F_4dd	G_1pd	G_3pd	G_1sp	G_2sd	W
d^2s^2	^3F	0	0	0	0	0	0	0	-8	-9	0	0	0	0	228.65
	^1D	0	0	0	0	0	0	0	-3	36	0	0	0	0	7,255.29
	^3P	0	0	0	0	0	0	0	7	-84	0	0	0	0	8,510.47
	^1G	0	0	0	0	0	0	0	4	1	0	0	0	0	12,118.46
d^3s	^5F	1	0	0	0	0	0	0	-15	-72	0	0	0	-3	6,680.49
	$^3F(2)$	1	0	0	0	0	0	0	-7.5	-36	0	0	0	-0.5	11,649.48
	^5P	1	0	0	0	0	0	0	0	-147	0	0	0	-3	14,038.63
	^3G	1	0	0	0	0	0	0	-11	13	0	0	0	-2	15,161.78
	$^3D(2)$	1	0	0	0	0	0	0	5	3	0	0	0	-2	17,444.67
	$^3P(2)$	1	0	0	0	0	0	0	-3	-6	0	0	0	0	18,067.56
	^3H	1	0	0	0	0	0	0	-6	-12	0	0	0	-2	18,127.71
	^1G	1	0	0	0	0	0	0	-11	13	0	0	0	0	18,287.62
	^1P	1	0	0	0	0	0	0	-6	-12	0	0	0	0	20,062.98
	$^1D(2)$	1	0	0	0	0	0	0	5	3	0	0	0	0	20,209.64
	^1H	1	0	0	0	0	0	0	-6	-12	0	0	0	0	20,795.65
d^3p	^5G	0	1	0	0	0	0	3	-23	-158	-4	-147	0	0	26,657.41
	$^3F(5)$	0	1	0	0	0	0	0.6	1.4	-28	-2.8	-32.4	0	0	34,393.76
	$^3D(6)$	0	1	0	0	0	0	.66	-.33	-52	-1.2	-21	0	0	38,970.97
	$^3G(4)$	0	1	0	0	0	0	.75	-5.7	-39.5	-1	-37	0	0	35,499.35
	^5F	0	1	0	0	0	0	3	-15	-72	-6	-78	0	0	28,703.00
	$^5D(2)$	0	1	0	0	0	0	-.5	-7.5	-109	-3.5	-78	0	0	32,742.21
	^5P	0	1	0	0	0	0	-7	0	-147	-1	-6.3	0	0	36,360.67
	$^3P(4)$	0	1	0	0	0	0	0	1	-38.3	-2.5	-41.2	0	0	39,833.85
	^5S	0	1	0	0	0	0	14	0	-147	-10	-105	0	0	37,359.13
	^3S	0	1	0	0	0	0	3	-6	-12	-9	-12	0	0	38,679.03
	^1I	0	1	0	0	0	0	-4	-6	-12	-10	-15	0	0	38,200.94
	^1S	0	1	0	0	0	0	1.25	-2.5	-28.6	-2	-1	0	0	41,172.38
	$^1G(3)$	0	1	0	0	0	0	2.33	1.33	-2	3	4	0	0	39,078.00
	$^3P(3)$ $H(3)$	0	1	0	0	0	0	-3.5	-8.5	0.5	-5	-30	0	0	39,157.14

Table 3 (cont'd). Multiple regression analysis input data for Ti I (cont'd)

Conf.	Multp.	ΔW_o					F_2pp	F_2pd	F_2dd	F_4dd	G_1pd	G_3pd	G_1sp	G_2sd	W
		(d^3s)	(d^3p)	(d^2sp)	(d^4)	(d^2p^2)									
d^3p (cont'd)	$^1D(4)$	0	1	0	0	0	0	-.75	3.25	-23.25	-.5	-16.5	0	0	42,258.55
	$^1F(4)$	0	1	0	0	0	0	0	2	-17	1.5	5	0	0	43,417.78
	^1I	0	1	0	0	0	0	3	-6	-12	-3	6	0	0	40,319.80
	$^3S(2)$	0	1	0	0	0	0	5	-3	-80	3	-6	0	0	42,851.04
	$^1H(2)$	0	1	0	0	0	0	-3.5	-3.5	0.5	2	6	0	0	42,601.58
d^2sp	^5G	0	0	1	0	0	0	1	-8	-9	-9	-12	-1	-2	16,106.08
	^5F	0	0	1	0	0	0	-3	-8	-9	-1	-48	-1	-2	16,981.42
	$^5D(2)$	0	0	1	0	0	0	0.5	-0.5	-46.5	-2	-58.5	-1	-2	22,141.97
	$^3F(4)$	0	0	1	0	0	0	.25	-3.75	4.75	-1	-21.75	-.5	-.75	28,108.15
	$^3D(5)$	0	0	1	0	0	0	1	-3	-30	-.8	-17.4	-.2	-.6	26,608.58
	$^3G(3)$	0	0	1	0	0	0	-3	-4	-5.66	-1	-8	-.33	-.66	27,688.04
	$^1D(3)$	0	0	1	0	0	0	1.33	-1.33	-19	0	10	-.33	.33	28,341.06
	$^1F(3)$	0	0	1	0	0	0	1.33	-2.33	9.33	-1	-13	.33	-.33	30,961.69
	$^1G(2)$	0	0	1	0	0	0	-5	-2	-4	3	-6	0	0	30,347.43
	$^3S(2)$	0	0	1	0	0	0	-14	7	-84	1.5	-10.5	0	-.5	30,180.31
	^5S	0	0	1	0	0	0	-14	7	-84	6	-42	-1	-2	25,102.88
	$^3P(4)$	0	0	1	0	0	0	2.75	6.25	-1.5	-1	-21.75	-.5	-.75	33,861.10
	^5P	0	0	1	0	0	0	7	7	-84	-6	-63	-1	-2	27,775.91
d^4	^5D	0	0	0	1	0	0	0	-2	-189	0	0	0	0	28,858.51
	^3P	0	0	0	1	0	0	0	-10	-153	0	0	0	0	34,352.96
	^3G	0	0	0	1	0	0	0	-12	-94	0	0	0	0	36,133.21
d^2p^2	$^5D(2)$	0	0	0	0	1	-5	-.5	-.5	-46.5	-5.5	-99	0	0	48,915.07
	$^1P(2)$	0	0	0	0	1	-2	-5	2	-24	1	-12	0	0	53,663.32
	^5F	0	0	0	0	1	-5	3	-8	-9	-8	-99	0	0	48,258.87
	^5F	0	0	0	0	1	-5	-1	-8	-9	-12	-51	0	0	47,189.86

Table 4. Multiple regression analysis input data for Ti II.

Conf.	Multp.	ΔW_0				F_2pd	F_2dd	F_4dd	G_1pd	G_3pd	G_1sp	G_2sd	W
		(ds^2)	(d^3)	(d^2p)	(dsp)								
d^2s	^4F	0	0	0	0	0	-8	-9	0	0	0	-2	224.98
	^2F	0	0	0	0	0	-8	-9	0	0	0	1	4,782.32
	^2D	0	0	0	0	0	-3	36	0	0	0	-1	8,726.47
	^4P	0	0	0	0	0	7	-84	0	0	0	-2	9,948.74
	^2G	0	0	0	0	0	4	1	0	0	0	-1	15,261.53
	^2P	0	0	0	0	0	7	-84	0	0	0	1	16,569.79
	^2S	0	0	0	0	0	14	126	0	0	0	-1	21,338.00
ds^2	^2D	1	0	0	0	0	0	0	0	0	0	0	25,066.34
d^3	^4F	0	1	0	0	0	-15	-72	0	0	0	0	1,048.61
	^2G	0	1	0	0	0	-11	13	0	0	0	0	9,058.15
	^4P	0	1	0	0	0	0	-147	0	0	0	0	9,425.84
	^2P	0	1	0	0	0	-6	-12	0	0	0	0	9,912.90
	^2H	0	1	0	0	0	-6	-12	0	0	0	0	12,725.99
	^2F	0	1	0	0	0	9	-87	0	0	0	0	20,921.88
d^2p	^4G	0	0	1	0	1	-8	-9	-9	-12	0	0	29,871.50
	^4F	0	0	1	0	-3	-8	-9	-1	-48	0	0	31,051.75
	$^2F(3)$	0	0	1	0	-1.33	-2.33	9.33	-1	-13	0	0	39,631.00
	$^4D(3)$	0	0	1	0	0.5	-0.5	-46.5	-2	-58.5	0	0	36,718.48
	$^2D(3)$	0	0	1	0	-1.33	-1.33	-19	0	10	0	0	38,613.00
	$^2G(2)$	0	0	1	0	-5	-2	-4	3	-6	0	0	39,202.68
	^2S	0	0	1	0	-14	7	-84	-3	21	0	0	37,430.55
	$^2P(3)$	0	0	1	0	1.33	6	26	.66	-8	0	0	42,574.00
	^4S	0	0	1	0	-14	7	-84	6	-42	0	0	40,027.28
	^4P	0	0	1	0	7	7	-84	-6	-63	0	0	42,235.85
	^2H	0	0	1	0	4	4	1	-6	-3	0	0	45,790.75
dsp	^4D	0	0	0	1	-7	0	0	3	-21	-1	-1	52,472.85
	$^2D(2)$	0	0	0	1	-7	0	0	0	0	0	0	61,526.00
	^4P	0	0	0	1	7	0	0	-1	-63	-1	-1	56,274.11
	^2F	0	0	0	1	2	0	0	0	0	0	0	65,072.07

Table 5. Multiple regression analysis input data for V I

Conf.	Multp.	ΔW_o					F_2pp	F_2pd	F_2dd	F_4dd	G_1pd	G_3pd	G_1sp	G_2sd	W
		(d^4s)	(d^5)	(d^3p^2)	(d^4p)	(d^3sp)									
d^3s^2	^4F	0	0	0	0	0	0	0	-15	-72	0	0	0	0	319.35
	^4P	0	0	0	0	0	0	0	0	-147	0	0	0	0	8,669.69
	^2G	0	0	0	0	0	0	0	-11	13	0	0	0	0	10,996.57
	^2P	0	0	0	0	0	0	0	-6	-12	0	0	0	0	13,806.53
	^2H	0	0	0	0	0	0	0	-6	-12	0	0	0	0	15,183.90
d^4s	^6D	1	0	0	0	0	0	0	-21	-189	0	0	0	-4	2,244.38
	^4H	1	0	0	0	0	0	0	-17	-69	0	0	0	-3	14,980.54
	^4G	1	0	0	0	0	0	0	-12	-94	0	0	0	-3	17,148.92
	^2P	1	0	0	0	0	0	0	-10	-153	0	0	0	0	18,997.16
	^2H	1	0	0	0	0	0	0	-17	-69	0	0	0	0	19,084.47
	^2F	1	0	0	0	0	0	0	-10	-153	0	0	0	-2	19,052.81
	$^4D(2)$	1	0	0	0	0	0	0	-10.5	-94.5	0	0	0	-1	14,673.49
d^5	^6S	0	1	0	0	0	0	0	-35	-315	0	0	0	0	20,202.49
	^4F	0	1	0	0	0	0	0	-13	-180	0	0	0	0	37,018.52
d^3p^2	^6G	0	0	1	0	0	-5	1	-15	-72	-17	-96	0	0	50,876.00
d^4p	^6P	0	0	0	1	0	0	-7	-21	-189	0	-105	0	0	24,738.17
	$^4P(4)$	0	0	0	1	0	0	-2.5	-9	-115.25	-3.5	-48	0	0	34,504.34
	^6F	0	0	0	1	0	0	-2	-21	-189	-10	-60	0	0	24,935.58
	^6D	0	0	0	1	0	0	7	-21	-189	-10	-105	0	0	26,570.88
	$^4S(2)$	0	0	0	1	0	0	4	-5	-76.5	-3.5	-78	0	0	36,408.23
	$^4H(2)$	0	0	0	1	0	0	-1.5	-14.5	-81.5	-8	-54	0	0	39,392.37
d^3sp	^6G	0	0	0	0	1	0	-1	-15	-72	-10	-30	-1	-3	16,694.36
	$^6D(2)$	0	0	0	0	1	0	-.5	-7.5	-109.5	-3.5	-78	-1	-3	23,412.55
	^6F	0	0	0	0	1	0	3	-15	-73	-6	-78	-1	-3	18,353.18
	$^4S(3)$	0	0	0	0	1	0	8	-2	-102	-1.33	-39	-.33	-1.33	37,146.00
	^6S	0	0	0	0	1	0	14	0	-147	-10	-105	-1	-3	30,832.58

Table 6. Multiple regression analysis input data for Vanadium II

Conf.	Multp.	ΔW_o			F_2pd	F_2dd	F_4dd	G_1pd	G_3pd	G_1sp	G_2sd	W
		(d^3s)	(d^2sp)	(d^3p)								
d^4	^5D	0	0	0	0	-21	-189	0	0	0	0	202.91
	$^3P(2)$	0	0	0	0	-5	-76.5	0	0	0	0	21,913.09
	^3H	0	0	0	0	-17	-69	0	0	0	0	12,625.57
	$^3F(2)$	0	0	0	0	-5	-76.5	0	0	0	0	21,925.04
	^3G	0	0	0	0	-12	-94	0	0	0	0	14,558.29
	$^1G(2)$	0	0	0	0	-5	-6.5	0	0	0	0	27,168.02
	$^1D(2)$	0	0	0	0	9	-76.5	0	0	0	0	31,484.93
	^1I	0	0	0	0	-15	-9	0	0	0	0	19,191.50
	$^1S(2)$	0	0	0	0	10	6	0	0	0	0	19,902.60
	^1F	0	0	0	0	0	-84	0	0	0	0	26,839.92
d^3s	^5F	1	0	0	0	-15	-72	0	0	0	-3	2,846.16
	^3F	1	0	0	0	-15	-72	0	0	0	-1	8,898.97
	^5P	1	0	0	0	0	-147	0	0	0	-3	13,616.00
	^3G	1	0	0	0	-11	13	0	0	0	-2	16,436.51
	^1G	1	0	0	0	-11	13	0	0	0	0	19,112.93
	^3H	1	0	0	0	-6	-12	0	0	0	-2	20,303.19
	$^3D(2)$	1	0	0	0	5	3	0	0	0	-2	32,373.38
	^1P	1	0	0	0	-6	-12	0	0	0	0	22,273.54
	^1H	1	0	0	0	-6	-12	0	0	0	0	23,391.09
	^1D	1	0	0	0	10	6	0	0	0	0	25,191.08
d^2sp	^5F	0	1	0	-3	-8	-9	-1	-48	-1	-2	63,827.00
	^5G	0	1	0	1	-8	-9	-9	-12	-1	-2	66,962.70
	^1H	0	1	0	4	4	1	-6	-3	1	-1	70,936.40
	$^5D(2)$	0	1	0	0.5	-0.5	-46.5	-2	-58.5	-1	-2	65,927.60
	$^1G(2)$	0	1	0	-5	-2	-4	3	-6	0	0	72,292.20

Table 6. (cont'd.)

Conf.	Multp.	ΔW_o (d^3s)	(d^2sp)	(d^3p)	F_2pd	F_2dd	F_4dd	G_1pd	G_3pd	G_1sp	G_2sd	W
d^3p	^5G	0	0	1	-1	-15	-72	-10	-30	0	0	34,992.30
	^5F	0	0	1	3	-15	-72	-6	-78	0	0	36,919.23
	^5D(2)	0	0	1	-0.5	-7.5	-109.5	-3.5	-78	0	0	42,260.00
	^3D(6)	0	0	1	-.66	-.33	-52	-1.16	-21	0	0	50,562.30
	^3G(4)	0	0	1	.75	-5.75	-52.75	-1.25	-36.75	0	0	51,897.13
	^3F(5)	0	0	1	0.6	-1.4	-28	-2.8	-32.4	0	0	56,067.32
	^3P(4)	0	0	1	0	1	-38.25	-2.5	-41.25	0	0	50,780.42
	^5P	0	0	1	-7	0	-147	-1	-63	0	0	46,904.94
	^3H(2)	0	0	1	-3.5	-8.4	0.5	-5	-30	0	0	49,750.04
	^1S	0	0	1	-4	-6	-12	-10	-15	0	0	48,258.28
	^1F(4)	0	0	1	0	2	-17	1.5	4.5	0	0	57,004.78
	^1H(2)	0	0	1	-3.5	-8.5	0.5	2	6	0	0	52,546.39
	^1G(3)	0	0	1	1.33	-2.66	-28.7	-2	-1	0	0	56,552.72
	^5S	0	0	1	14	0	-147	-10	-105	0	0	49,731.32
	^1D(4)	0	0	1	-0.75	3.25	-23.25	-0.5	-16.5	0	0	62,654.59
	^3S(2)	0	0	1	5	-3	-79.5	3	-6	0	0	53,922.22
	^1P(3)	0	0	1	2.33	1.33	-2	3	4	0	0	54,487.62
	^3I	0	0	1	3	-6	-12	-9	-12	0	0	53,098.92
	^1I	0	0	1	3	-6	-12	-3	6	0	0	55,403.38

Table 7. Multiple regression analysis input data for Cr I

Conf.	Multiplet	ΔW_o				F_2pd	F_2dd	F_4dd	G_1pd	G_3pd	G_1sp	G_2sd	W
		(d^4s^2)	(d^5)	(d^5p)	(d^4sp)								
d^5s	^7S	0	0	0	0	0	-35	-315	0	0	0	-5	0.00
	^5S	0	0	0	0	0	-35	-315	0	0	0	-1	7,593.16
	^5G	0	0	0	0	0	-25	-190	0	0	0	-4	20,523.69
	^5P	0	0	0	0	0	-28	-105	0	0	0	-4	21,847.88
	^5D	0	0	0	0	0	-18	-225	0	0	0	-4	24,299.89
	$^3G(3)$	0	0	0	0	0	-11.7	-163.4	0	0	0	-2	31,090.86
	$^3P(2)$	0	0	0	0	0	-4	-172.5	0	0	0	-1.5	27,190.22
	$^3D(4)$	0	0	0	0	0	-7	-131	0	0	0	-2.3	29,855.25
	^3I	0	0	0	0	0	-24	-90	0	0	0	-3	31,049.23
	^5F	0	0	0	0	0	-13	-180	0	0	0	-4	31,364.33
	$^3F(3)$	0	0	0	0	0	-16	-120	0	0	0	-2	35,157.87
	^1I	0	0	0	0	0	-24	-90	0	0	0	-1	33,762.74
	^3H	0	0	0	0	0	-22	-30	0	0	0	-3	35,903.00
	^1H	0	0	0	0	0	-22	-30	0	0	0	-1	38,537.68
	$^1G(2)$	0	0	0	0	0	-5	-150	0	0	0	-1	39,158.63
d^4s^2	^5D	1	0	0	0	0	-21	-189	0	0	0	0	8,037.47
	$^3P(2)$	1	0	0	0	0	-5	-76.5	0	0	0	0	23,632.00
	^3H	1	0	0	0	0	-17	-69	0	0	0	0	24,067.11
	$^3F(2)$	1	0	0	0	0	-5	-76.5	0	0	0	0	25,059.14
	^3G	1	0	0	0	0	-12	-94	0	0	0	0	27,703.84
	$^1G(2)$	1	0	0	0	0	-5	-6.5	0	0	0	0	31,987.06
	^1I	1	0	0	0	0	-15	-9	0	0	0	0	32,097.36
	$^3D(2)$	1	0	0	0	0	-5	-129	0	0	0	0	33,920.65
d^6	^5D	0	1	0	0	0	-21	-189	0	0	0	0	35,520.48
d^5p	^7P	0	0	1	0	0	-35	-315	-10	-105	0	0	23,401.35
	$^5P(3)$	0	0	1	0	0	-27	-215	-3.3	-55	0	0	40,227.10
	$^5G(2)$	0	0	1	0	0	-19	-189	-10	-82.5	0	0	49,422.21
	$^3H(5)$	0	0	1	0	0	-16.2	-122	-5.8	-47.4	0	0	56,646.10

Table 7. (cont'd)

Config.	Multip.	ΔW_o (d^4s^2)	(d^5)	(d^5p)	(d^4sp)	F_2pd	F_2dd	F_4dd	G_1pd	G_3pd	G_1sp	G_2sd	W
d^5p (cont'd)	^5H	0	0	1	0	0	-25	-190	-10	-60	0	0	45,663.28
	$^3P(3)$	0	0	1	0	0	-13	-355	-8.3	-135	0	0	51,229.56
	$^5D(3)$	0	0	1	0	0	-19.7	-170	-6.6	-90	0	0	47,067.80
	$^5F(3)$	0	0	1	0	0	-15.3	-198.3	-6.6	-90	0	0	49,132.79
	$^3S(2)$	0	0	1	0	0	-4	-172	3	-28.5	0	0	49,477.04
	^5S	0	0	1	0	0	-28	-105	-10	-105	0	0	49,822.59
	$^1H(4)$	0	0	1	0	0	-14	-105	-1.75	-20.25	0	0	55,703.42
	$^3I(2)$	0	0	1	0	0	-23	-60	-8	-54	0	0	56,272.43
	^3K	0	0	1	0	0	-24	-90	-10	-30	0	0	54,404.94
	^1K	0	0	1	0	0	-24	-90	-8	6	0	0	54,970.23
	$^1I(2)$	0	0	1	0	0	-23	-60	-2	-6	0	0	57,979.05
d^4sp	^7F	0	0	0	1	-2	-21	-189	-10	-60	-1	-4	25,206.02
	^7D	0	0	0	1	7	-21	-189	-10	-105	-1	-4	27,500.37
	^7P	0	0	0	1	-7	-21	-189	0	-105	-1	-4	27,820.23
	$^5P(5)$	0	0	0	1	-3.4	-11.4	-132	-2.8	-59.4	-.6	-2.4	40,612.57
	$^5H(2)$	0	0	0	1	-1.5	-14.5	-81.5	-8	-54	-1	-3	44,973.78
	$^5S(2)$	0	0	0	1	4	-5	-76.5	-3.5	-78	-1	-3	43,124.88
	^5I	0	0	0	1	1	-17	-69	-10	-30	-1	-3	44,458.00
	$^5G(4)$	0	0	0	1	1.2	-9.7	-79	-5.7	-66	-1	-3	47,098.67
	$^3S(4)$	0	0	0	1	4	-5	-76.5	-3.5	-44.2	0	-1.5	53,586.00
	$^3I(3)$	0	0	0	1	-1	-16.4	-49	-5.4	-21	-.33	-5.6	54,632.67
	$^1I(2)$	0	0	0	1	-2	-16	-39	-3	-16.5	=0	-1	54,800.06
	$^1H(5)$	0	0	0	1	0	-10.8	-37	-2	-21	0.2	-1.2	55,945.08

Table 3. Multiple regression analysis input data for Cr II

Conf.	Multp.	ΔW_o			F_2pd	F_2dd	F_4dd	G_1pd	G_3pd	G_2sd	W
		(d^4s)	(d^3s^2)	(d^4p)							
d^5	^6S	0	0	0	0	-35	-315	0	0	0	0.00
	^4G	0	0	0	0	-25	-190	0	0	0	20,518.33
	^4P	0	0	0	0	-28	-105	0	0	0	21,824.82
	^4D	0	0	0	0	-18	-225	0	0	0	25,043.10
	^2I	0	0	0	0	-24	-90	0	0	0	30,146.72
	$^2D(3)$	0	0	0	0	-3.33	-100	0	0	0	39,401.57
	$^2F(2)$	0	0	0	0	-17	-90	0	0	0	36,142.00
	^4F	0	0	0	0	-13	-180	0	0	0	32,855.00
	^2H	0	0	0	0	-22	-30	0	0	0	35,658.90
	$^2G(2)$	0	0	0	0	-5	-150	0	0	0	44,242.00
	^2S	0	0	0	0	-3	-195	0	0	0	44,307.44
d^4s	^6D	1	0	0	0	-21	-189	0	0	-4	12,228.00
	$^4D(2)$	1	0	0	0	-13	-159	0	0	-1	29,054.50
	$^4P(2)$	1	0	0	0	-5	-76.5	0	0	-3	30,407.00
	^4H	1	0	0	0	-17	-69	0	0	-3	30,298.77
	$^4F(2)$	1	0	0	0	-5	-76.5	0	0	-3	31,168.78
	^4G	1	0	0	0	-12	-94	0	0	-3	33,553.24
	^2H	1	0	0	0	-17	-69	0	0	0	34,722.14
	$^2P(2)$	1	0	0	0	-5	-76.5	0	0	0	35,002.00
	$^2F(3)$	1	0	0	0	-3.3	-51	0	0	-2	43,132.00
	^2I	1	0	0	0	-15	-9	0	0	-2	40,215.00
	$^2S(2)$	1	0	0	0	10	6	0	0	-2	40,415.34
d^3s^2	^4F	0	1	0	0	-15	-72	0	0	0	53,452.75
	^2G	0	1	0	0	-11	13	0	0	0	54,561.19
	^4P	0	1	0	0	0	-147	0	0	0	55,052.50
	^2P	0	1	0	0	-6	-12	0	0	0	59,130.51
	^2D	0	1	0	0	5	3	0	0	0	59,538.50

Table 8. (cont'd)

Conf.	Multp.	ΔW_o (d^4s)	(d^3s^2)	(d^4p)	F_2pd	F_2dd	F_4dd	G_1pd	G_3pd	G_2sd	W
d^4p	^6F	0	0	1	-2	-21	-189	-10	-60	0	47,227.50
	^6P	0	0	1	-7	-21	-189	0	-105	0	48,516.39
	$^4P(4)$	0	0	1	-2.5	-9	-117	-3.5	-48	0	63,409.66
	^6D	0	0	1	7	-21	-189	-10	-105	0	49,706.47
	$^4F(5)$	0	0	1	-1.8	-9.6	-113	-2.8	-53.4	0	65,762.00
	$^4D(6)$	0	0	1	2	-7.66	-104	-4	-54.5	0	65,079.75
	$^4H(2)$	0	0	1	-1.5	-14.5	-81.5	-8	-54	0	66,464.00
	$^2S(2)$	0	0	1	4	-5	-76.5	-3.5	-10.5	0	65,029.67
	$^4G(4)$	0	0	1	1.25	-9.75	-79	-5.75	-66	0	67,805.53
	^4I	0	0	1	1	-17	-69	-10	-30	0	65,519.95
	$^2G(7)$	0	0	1	1.14	-7	-59	-2.42	-18	0	75,021.20
	$^2D(8)$	0	0	1	1.9	-0.9	-84	-.625	-26.25	0	78,812.17
	$^2P(7)$	0	0	1	-1	3.3	-60.4	-0.71	-30	0	75,630.50
	$^2I(2)$	0	0	1	-2	-16	-39	-3	-16.5	0	70,984.67
	$^4S(2)$	0	0	1	4	-5	-76.5	-3.5	-78	0	68,305.73
	$^2H(5)$	0	0	1	0	-10.8	-37	-2	-21	0	76,031.00
	^2F	0	0	1	-1.7	-2.1	-69.6	-1.2	-28.1	0	76,093.70

Table 9. Multiple regression analysis input data for Mn I

Conf.	Multp.	ΔW_o					F_2pd	F_2dd	F_4dd	G_1pd	G_3pd	G_1sp	G_2sd	W
		(d^6s)	(d^6p)	(d^7)	(d^5p^2)	(d^5sp)								
d^5s^2	^6S	0	0	0	0	0	0	-35	-315	0	0	0	0	0.00
	^4G	0	0	0	0	0	0	-25	-190	0	0	0	0	25,280.06
	^4P	0	0	0	0	0	0	-28	-105	0	0	0	0	27,243.80
	^4D	0	0	0	0	0	0	-18	-225	0	0	0	0	30,402.80
d^6s	^6D	1	0	0	0	0	0	-21	-189	0	0	0	-4	17,398.29
	$^4D(2)$	1	0	0	0	0	0	-13	-159	0	0	0	-2	23,596.07
	$^4P(2)$	1	0	0	0	0	0	-5	-76.5	0	0	0	-3	34,378.04
	^4H	1	0	0	0	0	0	-17	-69	0	0	0	-3	34,289.14
	$^4F(2)$	1	0	0	0	0	0	-5	-76.5	0	0	0	-3	35,065.03
	^4G	1	0	0	0	0	0	-12	-94	0	0	0	-3	37,644.56
	^2H	1	0	0	0	0	0	-17	-69	0	0	0	0	38,064.44
	$^2F(3)$	1	0	0	0	0	0	-3.3	-79	0	0	0	-.66	38,669.60
d^6p	^6F	0	1	0	0	0	2	-21	-189	-24	-252	0	0	43,500.00
	^6D	0	1	0	0	0	-7	-21	-189	-24	-252	0	0	42,023.00
	^6P	0	1	0	0	0	7	-21	-189	-24	-252	0	0	45,136.34
	$^4P(4)$	0	1	0	0	0	2.5	-9	-118	-19	-230	0	0	53,251.00
	$^4G(4)$	0	1	0	0	0	-1.2	-9.7	-79	-21.5	-229.	0	0	58,920.50
	$^4H(2)$	0	1	0	0	0	1.5	-14.5	-81.5	-24	-229.5	0	0	58,427.30
	^4I	0	1	0	0	0	-1	-17	-69	-24	-207	0	0	58,851.49
	$^2I(2)$	0	1	0	0	0	2	-16	-39	-21.5	-176	0	0	59,722.50
d^7	^4F	0	0	1	0	0	0	-15	-72	0	0	0	0	45,045.63
	^4P	0	0	1	0	0	0	0	-147	0	0	0	0	51,714.34
d^5p^2	^8P	0	0	0	1	0	0	-35	-315	-20	-210	0	0	57,231.13
d^5sp	^8P	0	0	0	0	1	0	-35	-315	-10	-105	-1	-5	18,556.64
	$^6P(4)$	0	0	0	0	1	0	-29	-240	-5	-67	-.5	-3	42,062.92
	$^6D(3)$	0	0	0	0	1	0	-20	-170	-6.6	-90	-1	-4	54,466.39
	$^6F(3)$	0	0	0	0	1	0	-18.6	-198	-6.6	-90	-1	-4	49,620.47
	$^4S(3)$	0	0	0	0	1	0	-12	-150	-1.3	-54	-.33	-2.3	55,864.44
	$^4I(2)$	0	0	0	0	1	0	-23	-60	-8	-54	-1	-3	61,225.55

Table 10. Multiple regression analysis input data for Mn II

Conf.	Multp.	ΔW_0 (d^5s)	(d^5p)	(d^4s^2)	(d^4sp)	F_2pd	F_2dd	F_4dd	G_1pd	G_3pd	G_1sp	G_2sd	W
d^6	^5D	0	0	0	0	0	-21	-189	0	0	0	0	14,781.03
	$^3P(2)$	0	0	0	0	0	-5	-76.5	0	0	0	0	30,276.96
	^3H	0	0	0	0	0	-17	-69	0	0	0	0	30,679.24
	$^3F(2)$	0	0	0	0	0	-5	-76.5	0	0	0	0	31,636.72
	^3G	0	0	0	0	0	-12	-94	0	0	0	0	33,209.39
	^3D	0	0	0	0	0	-5	-129	0	0	0	0	37,833.90
d^5s	^7S	1	0	0	0	0	-35	-135	0	0	0	-5	0.00
	^5S	1	0	0	0	0	-35	-135	0	0	0	-1	9,472.86
	^5G	1	0	0	0	0	-25	-190	0	0	0	-4	27,570.95
	^5P	1	0	0	0	0	-28	-105	0	0	0	-4	29,951.12
	^5D	1	0	0	0	0	-18	-225	0	0	0	-4	32,818.10
	$^3G(2)$	1	0	0	0	0	-5	-150	0	0	0	-3	34,910.43
	$^3P(2)$	1	0	0	0	0	-14	-52.5	0	0	0	-1.5	36,350.30
	$^3D(4)$	1	0	0	0	0	-4.5	-55.2	0	0	0	-2.2	39,813.38
	^5F	1	0	0	0	0	-13	-180	0	0	0	-4	43,395.00
d^5p	^7P	0	1	0	0	0	-35	-315	-10	-105	0	0	38,571.85
	$^5P(3)$	0	1	0	0	0	-27	-215	-3.3	-53	0	0	61,068.00
	$^5G(2)$	0	1	0	0	0	-19	-185	-10	-82.5	0	0	64,493.83
	^5H	0	1	0	0	0	-25	-190	-10	-60	0	0	65,658.30
	$^5F(3)$	0	1	0	0	0	-15.3	-198	-6.6	-90	0	0	68,571.11
	$^5D(3)$	0	1	0	0	0	-19.6	-170	-6.66	-90	0	0	69,635.80
	^5S	0	1	0	0	0	-28	-105	-10	-105	0	0	66,929.22
	$^3H(5)$	0	1	0	0	0	-16.2	-122	-5.8	-46	0	0	67,825.93
	$^3S(2)$	0	1	0	0	0	-4	-172	3	-28.5	0	0	73,911.00
d^4s^2	^5D	0	0	1	0	0	-21	-189	0	0	0	0	55,193.20
d^4sp	^7P	0	0	0	1	-7	-21	-189	0	-105	-1	-4	83,391.60
	$^5P(5)$	0	0	0	1	-3.4	-11.4	-132	-2.8	-59	-.6	-2.4	102,335.33
	$^5H(2)$	0	0	0	1	-1.5	-14.5	-81	-8	-54	-1	-3	110,692.20
	$^5G(4)$	0	0	0	1	1.2	-9.7	-79	-5.7	-66	-1	-3	113,181.70

Table 11. Multiple regression analysis input data for Fe I

Conf.	Multp.	ΔW_o			F_2pd	F_2dd	F_4dd	G_1pd	G_3pd	G_2sd	W
		(d^7s)	(d^7p)	(d^6sp)							
d^6s^2	^1I	0	0	0	0	-15	-9	0	0	0	29,313.04
	^3H	0	0	0	0	-17	-69	0	0	0	19,575.71
	^3G	0	0	0	0	-12	-94	0	0	0	24,039.32
	^5D	0	0	0	0	-21	-180	0	0	0	402.96
	^3D	0	0	0	0	-5	-129	0	0	0	29,356.47
d^7s	^3H	1	0	0	0	-6	-12	0	0	-2	26,329.94
	^1H	1	0	0	0	-6	-12	0	0	0	28,819.89
	^3G	1	0	0	0	-11	13	0	0	-2	21,948.60
	^1G	1	0	0	0	-11	13	0	0	0	24,574.69
	^5F	1	0	0	0	-15	-72	0	0	-3	7,459.76
(^4F)	^3F	1	0	0	0	-15	-72	0	0	1	12,407.42
(^2F)	^3F	1	0	0	0	9	-87	0	0	-2	36,997.45
	^1F	1	0	0	0	9	-87	0	0	0	40,534.18
	^5P	1	0	0	0	0	-147	0	0	-3	17,684.59
(^4P)	^3P	1	0	0	0	0	-147	0	0	1	22,988.24
(^2P)	^3P	1	0	0	0	-6	-12	0	0	-2	24,565.20
	^1P	1	0	0	0	-6	-12	0	0	0	27,543.00
d^7p	^3I	0	1	0	-3	-6	-12	-18	-144	0	52,676.72
	^1I	0	1	0	-3	-6	-12	-18	-84	0	53,077.91
	$^3H(2)$	0	1	0	3.5	-8.5	0.5	-18	-166.5	0	51,077.91
	$^1H(2)$	0	1	0	3.5	-8.5	0.5	-14	-109.5	0	51,052.54
	^5G	0	1	0	1	-15	-72	-18	-189	0	35,143.52
	^5F	0	1	0	-3	-15	-72	-18.5	-189	0	34,117.70
	$^5D(2)$	0	1	0	0.5	-7.5	-109.5	-18	-189	0	40,168.87
	^5P	0	1	0	7	0	-147	-18	-189	0	48,096.90
	^5S	0	1	0	-14	0	-147	-18	-189	0	44,511.86
	$^3S(2)$	0	1	0	-5	-3	-79.5	-5	-135	0	50,206.74
d^6sp	^7F	0	0	1	2	-21	-189	-24	-252	-4	22,928.05
	^7D	0	0	1	-7	-21	-189	-24	-252	-4	19,624.08
	^7P	0	0	1	7	-21	-189	-24	-252	-4	24,057.33

Table 12. Multiple regression analysis input data for Fe II

Conf.	Multp.	ΔW_o			F_2pd	F_2dd	F_4dd	G_1pd	G_3pd	G_2sd	W
		(d^6s)	(d^5s^2)	(d^6p)							
d^7	^2H	0	0	0	0	-6	-12	0	0	0	20,551.94
	^2G	0	0	0	0	-11	13	0	0	0	16,077.90
	^4F	0	0	0	0	-15	-72	0	0	0	2,416.58
	^2F	0	0	0	0	9	-87	0	0	0	31,918.87
	$^2D(2)$	0	0	0	0	5	3	0	0	0	34,363.43
	^4P	0	0	0	0	0	-147	0	0	0	13,612.43
	^2P	0	0	0	0	-6	-12	0	0	0	18,536.02
d^6s	^2I	1	0	0	0	-15	-9	0	0	-2	32,891.43
	^4H	1	0	0	0	-17	-69	0	0	-3	21,459.04
	^2H	1	0	0	0	-17	-69	0	0	0	26,253.19
	^4G	1	0	0	0	-12	-94	0	0	-3	25,760.68
	$^2G(3)$	1	0	0	0	-7.33	-35.67	0	0	-1.33	40,894.89
(^3F)	$^4F(2)$	1	0	0	0	-5	-76.5	0	0	-3	36,479.60
(^3F)	$^2F(2)$	1	0	0	0	-5	-76.5	0	0	0	41,167.91
(^1F)	$^2F(2)$	1	0	0	0	0	-84	0	0	-2	44,921.29
	^6D	1	0	0	0	-21	-189	0	0	-4	496.29
(^5D)	^4D	1	0	0	0	-21	-189	0	0	1	8,846.76
(^3D)	^4D	1	0	0	0	-5	-129	0	0	-2	31,419.41
(^3D)	^2D	1	0	0	0	-5	-129	0	0	0	36,202.34
	$^4P(2)$	1	0	0	0	-5	-76.5	0	0	-3	35,606.61
	$^2P(2)$	1	0	0	0	-5	-76.5	0	0	0	40,396.05
d^5s^2	^4D	0	1	0	0	-18	-225	0	0	0	60,368.29
	^6S	0	1	0	0	-35	-315	0	0	0	23,317.60
d^6p	^2K	0	0	1	-2	-15	-9	-24	-177	0	71,224.59
	^4I	0	0	1	-1	-17	-69	-24	-207	0	61,483.06
	$^2I(2)$	0	0	1	-2	-16	-39	-21.5	-177	0	68,215.89
	$^4H(2)$	0	0	1	1.5	-14.5	-81.5	-24	-229.5	0	63,728.70
	^6F	0	0	1	2	-21	-189	-24	-252	0	42,156.09
	$^4F(5)$	0	0	1	1.8	-9.6	-113	-21.2	-213.6	0	67,804.22
	^6D	0	0	1	-7	-21	-189	-24	-252	0	38,709.86
	^6P	0	0	1	7	-21	-189	-25	-252	0	43,065.63

Table 13. Multiple regression analysis input data for Co. I.

Conf.	Multp.	ΔW_o				F_2pd	F_2dd	F_4dd	G_1pd	G_3pd	G_1sp	G_2sd	W
		(d^9)	(d^8s)	(d^8p)	(d^7sp)								
d^7s^2	^2H	0	0	0	0	0	-6	-12	0	0	0	0	22,127.91
	^2G	0	0	0	0	0	-11	13	0	0	0	0	16,850.79
	^4F	0	0	0	0	0	-15	-7	0	0	0	0	793.08
	^4P	0	0	0	0	0	0	-147	0	0	0	0	14,010.36
	^2P	0	0	0	0	0	-6	-12	0	0	0	0	20,858.31
d^9	^2D	1	0	0	0	0	0	0	0	0	0	0	27,983.78
d^8s	^4F	0	1	0	0	0	-8	-9	0	0	0	-2	4,347.87
	^2F	0	1	0	0	0	-8	-9	0	0	0	1	7,951.61
	^4P	0	1	0	0	0	7	-84	0	0	0	-2	15,717.92
	^2P	0	1	0	0	0	7	-84	0	0	0	1	18,582.29
	^2D	0	1	0	0	0	-3	36	0	0	0	-1	22,526.33
d^8p	^2H	0	0	1	0	-4	4	1	-12	-81	0	0	50,293.36
	^4G	0	0	1	0	-1	-8	-9	-12	-126	0	0	32,935.76
	^4F	0	0	1	0	3	-8	-9	-12	-126	0	0	33,612.74
	^4P	0	0	1	0	-7	7	-84	-12	-126	0	0	44,665.25
	^4S	0	0	1	0	14	7	-84	-12	-126	0	0	48,753.72
	^2S	0	0	1	0	14	7	-84	-12	-126	0	0	47,977.94
d^7sp	^6G	0	0	0	1	1	-15	-72	-18	-189	-3	-3	25,987.48
	^6F	0	0	0	1	-3	-15	-72	-18	-189	-3	-3	24,466.79
	$^6D(2)$	0	0	0	1	0.5	-7.5	-109.5	-18	-189	-3	-3	25,590.11
	$^2H(4)$	0	0	0	1	3.5	-8.5	0.5	-16	-138	-2	-1	48,064.36
	$^4S(3)$	0	0	0	1	-8	-2	-102	-9.3	-153	-2.3	-1.3	43,592.25

Table 14. Multiple regression analysis input data for Co II

Conf.	Multp.	ΔW_o				F_2pd	F_2dd	F_4dd	G_1pd	G_3pd	G_1sp	G_2sd	W
		(d^6s^2)	(d^7s)	(d^7p)	(d^6sp)								
d^8	^3F	0	0	0	0	0	-8	-9	0	0	0	0	671.70
	^3P	0	0	0	0	0	7	-84	0	0	0	0	13,419.73
d^6s^2	^5D	1	0	0	0	0	-21	-189	0	0	0	0	41,438.80
d^7s	^5F	0	1	0	0	0	-15	-72	0	0	0	-3	4,110.33
	^3F	0	1	0	0	0	-15	-72	0	0	0	1	10,446.46
	^5P	0	1	0	0	0	0	-147	0	0	0	-3	18,047.17
(^4P)	^3P	0	1	0	0	0	0	-147	0	0	0	1	24,251.30
(^2P)	^3P	0	1	0	0	0	-6	-12	0	0	0	-2	24,886.50
	^3D	0	1	0	0	0	10	6	0	0	0	-2	27,727.17
d^7p	^5G	0	0	1	0	1	-15	-72	-18	-189	0	0	47,753.98
	^5F	0	0	1	0	-3	-15	-72	-18	-189	0	0	45,957.52
	^5P	0	0	1	0	7	0	-147	-18	-189	0	0	63,458.67
	^5S	0	0	1	0	-14	0	-147	-18	-189	0	0	56,010.60
d^6sp	$^5D(7)$	0	0	0	1	-2.71	-9.57	-116.15	-19.29	-227	-2.7	-2.57	80,733.76
	$^5F(6)$	0	0	0	1	1.83	-11.5	-125.7	-21.7	-220	-2.67	-2.5	82,314.33
	$^5P(5)$	0	0	0	1	3.4	-11.4	-123	-20.2	-234.6	-2.6	-2.4	85,630.43

Table 15. Multiple regression analysis input data for Ni I

Conf.	Multp.	ΔW_o (d^9p)	(d^8s^2)	(d^8sp)	F_2pd	F_2dd	F_4dd	G_1pd	G_3pd	G_1sp	G_2sd	W
d^9s	^3D	0	0	0	0	0	0	0	0	0	-1	681.18
	^1D	0	0	0	0	0	0	0	0	0	1	3,409.92
d^9p	^3F	1	0	0	-2	0	0	-6	-63	0	0	29,680.59
	^1F	1	0	0	-2	0	0	-6	27	0	0	31,031.04
	^3D	1	0	0	7	0	0	-6	-63	0	0	29,949.43
	^1D	1	0	0	7	0	0	-6	-63	0	0	31,441.66
	^3P	1	0	0	-7	0	0	-6	-63	0	0	29,207.28
	^1P	1	0	0	-7	0	0	14	-63	0	0	32,982.28
d^8s^2	^1G	0	1	0	0	4	1	0	0	0	0	22,102.35
	^3F	0	1	0	0	-8	-9	0	0	0	0	936.61
	^1D	0	1	0	0	-3	36	0	0	0	0	13,742.76
	^3P	0	1	0	0	7	-84	0	0	0	0	15,744.75
d^8sp	^5G	0	0	1	-1	-8	-9	-12	-126	-3	-2	27,875.02
	^5F	0	0	1	3	-8	-9	-12	-126	-3	-2	29,284.35
	$^1G(2)$	0	0	1	10	-4	-8	-24	-132	-4	0	33,590.16
	$^5D(2)$	0	0	1	-1	-1	-93	-12	-126	-3	-2	26,726.12

Table 16. Multiple regression analysis input data for Ni II

Conf.	Multp.	$\Delta W_o(d^8s)$	$\Delta W_o(d^8p)$	F_2pd	F_2dd	F_4dd	G_1pd	G_3pd	G_2sd	W
d^9	^2D	0	0	0	0	0	0	0	0	603.76
d^8s	^2G	1	0	0	4	1	0	0	-1	32,511.40
	^4F	1	0	0	-8	-9	0	0	-2	9,354.90
	^2F	1	0	0	-8	-9	0	0	1	14,169.71
	^4P	1	0	0	7	-84	0	0	-2	24,386.60
	^2P	1	0	0	7	-84	0	0	1	29,244.77
	^2D	1	0	0	-3	36	0	0	-1	23,383.30
d^8p	^2H	0	1	-4	4	1	-12	-81	0	75,461.60
	^4G	0	1	-1	-8	-9	-12	-126	0	54,035.87
	^4F	0	1	3	-8	-9	-12	-126	0	55,618.50
	^4P	0	1	-7	7	-84	-12	-126	0	66,651.12
	^4S	0	1	14	7	-84	-12	-126	0	74,300.30
	^2S	0	1	14	7	-84	-12	-126	0	74,283.00

Table 17. Spectroscopic data for Cu I

Conf.	Multp.	G_1pd	G_3pd	G_1sp	G_2sd	W
d^9sp	^4F	-6	-63	-3	-1	40,687.07
	$^2F(2)$	-6	-16	-2	0	50,048.22
	^4D	-6	-63	-3	-1	41,919.35
	$^2D(2)$	-6	-63	-2	0	49,740.98
	^4P	-6	-63	-3	-1	41,913.11
	$^2P(2)$	-6	-63	-2	0	53,647.13
$d^{10}s$	^2S					0.00
d^9s^2	^2D					12,019.70
$d^{10}p$	^2P					30,700.89

Table 18. Multiple regression analysis input data for Cu II

Conf.	Multp.	$\Delta W_o(d^9p)$	$\Delta W_o(d^8s^2)$	$\Delta W_c(d^8sp)$	F_2pd	F_2dd	F_4dd	G_1pd	G_3pd	G_1sp	G_2sd	W
d^9s	^3D	0	0	0	0	0	0	0	0	0	-1	22,580.03
	^1D	0	0	0	0	0	0	0	0	0	1	26,264.52
d^9p	^3F	1	0	0	-2	0	0	-6	-63	0	0	69,000.31
	^1F	1	0	0	-2	0	0	-6	27	0	0	71,920.13
	^3D	1	0	0	7	0	0	-6	-63	0	0	71,435.74
	^1D	1	0	0	7	0	0	-6	-63	0	0	73,353.43
	^3P	1	0	0	-7	0	0	-6	-63	0	0	67,083.22
	^1P	1	0	0	-7	0	0	14	-63	0	0	73,595.86
d^8s^2	^1G	0	1	0	0	4	1	0	0	0	0	95,565.65
	^3F	0	1	0	0	-8	-9	0	0	0	0	70,984.63
	^1D	0	1	0	0	-3	36	0	0	0	0	85,388.77
	^3P	0	1	0	0	7	-84	0	0	0	0	88,537.08
d^8sp	^3H	0	0	1	-4	4	1	-12	-81	-3	-1	136,694.10
	^1H	0	0	1	-4	4	1	-12	-81	-1	-1	137,082.50
	^5G	0	0	1	-1	-8	-9	-12	-126	-3	-3	111,322.29
	^5F	0	0	1	3	-8	-9	-12	-126	-3	-2	113,893.26
	^5P	0	0	1	-7	7	-84	-12	-126	-3	-2	129,136.15
	^5S	0	0	1	14	7	-84	-12	-126	-4	-1	128,365.70

Table 19. Multiple regression analysis input data for Zn I and II

Zn I

Config.	Multiplet	$\Delta W_o(sp)$	$W_o(p^2)$	F_2pp	G_1sp	W cm^{-1}
s^2	^1S	0	0	0	0	0.00
sp	^1P	1	0	0	1	46,745.47
	^3P	1	0	0	-1	32,567.67
p^2	^1D	0	1	1	0	80,795.00
	^3P	0	1	-5	0	80,285.00
	^1S	0	1	10	0	81,561.07

Zn II

Config.	Multiplet	W
s	^2S	0.00
p	^2P	48,917.50

Table 20. Multiple regression analysis input data for Ga I and II

Ga I

Config.	Multiplet	$\Delta W_o(sp^2)$	$F_2(pp)$	$G_1(sp)$	W
s^2p	^2S	0	0	0	0.00
	^2P	0	0	0	826.24
sp^2	^2P	1	-5	1	66,109.00
	^4P	1	-5	-2	38,407.70
	^2S	1	10	-1	62,100.00

Ga II

Config.	Multiplet	$\Delta W_o(sp)$	$\Delta W_o(p^2)$	F_2pp	G_1sp	W
s^2	^1S	0	0	0	0	0.00
sp	^1P	1	0	0	1	70,700.00
	^3P	1	0	0	-1	47,978.70
p^2	^3P	0	1	-5	0	115,354.30

Table 21. Multiple regression analysis input data for Ge I and II

Ge I

Config.	Multiplet	$\Delta W_o(sp^3)$	F_2pp	G_1sp	W
s^2p^2	^3P	0	-5	0	1,125.63
	^1D	0	1	0	7,125,26
	^1S	0	10	0	16,367,14
sp^3	^1P	1	0	0	55,473,60
	^3P	1	0	-2	57,098,00
	^1D	1	-6	0	58,091,30
	^3D	1	-6	-2	59,677.70

Ge II

Config.	Multiplet	$\Delta W_o sp^2$	$\Delta W_o p^3$	F_2pp	$G_1 sp$	W
s^2p	^2P	0	0	0	0	1,178,06
sp^2	^4P	1	0	-5	-2	52,709.44
	^2P	1	0	1	+1	65,116.44
	^2D	1	0	10	-1	85,889.90
	^2S	1	0	-5	1	91,753.00
p^3	^4S	0	1	-15	0	136,273.30

Table 22. Multiple regression analysis input data for As I and II

As I

Config.	Multiplet	$\Delta W_o(sp^4)$	F_2pp	G_1sp	W
s^2p^3	^4S	0	-15	0	0.00
	^2D	0	-6	0	10,753.55
	^2P	0	0	0	18,416.80
sp^4	^4P	1	-5	-3	56,572.70
	^2P	1	-5	0	65,154.45
	^2D	1	1	-2	68,351.65

As III

Config.	Multiplet	$\Delta W_o(sp^3)$	F_2pp	G_1sp	W
s^2p^2	^3P	0	-5	0	1,535.25
	^1D	0	1	0	10,093.00
	^1S	0	10	0	22,593.00
sp^3	^3D	1	-6	-2	73,950.00
	^1P	1	0	0	83,099.00
	^3P	1	0	-2	84,730.67

Table 23. Multiple regression analysis input data for Se and II

Se I

Config.	Multiplet	F_2pp	G_1sp	W
s^2p^4	^3P	-5	0	1,130.96
	^1D	1	0	9,576.08
	^1S	10	0	22,556.03

Se II

Config.	Multiplet	$\Delta W_0(sp^4)$	F_2pp	G_1sp	W
s^2p^3	^4S	0	-15	0	0.00
	^2D	0	-6	0	13,476.60
	^2P	0	0	0	23,466.55
sp^4	^4P	1	-5	-3	84,871.13
	^2P	1	-5	0	100,295.10

Table 24. Spectroscopic data for Br I and II

Br I

Isoelectronic elements	$^2P, s^2p^5$	$^2S, sp^6$
BrI	1,228.33	---
Kr II	1,790.33	109,002.06
Rb III	2,460.00	130,036.00
Sr IV	3,243.37	150,505.00
Y V	4,032.67	170.936.00

Br II

Config.	Multiplet	F_2pp	G_1sp	W
s^2p^4	^3P	-5	0	1,747.50
	^1D	1	0	11,409.00
sp^5	^3P	0	-1	97,228.71

Table 25. Parameters for C I and C II

C I		C II	
D. F. @	3/4	D.F. @	3/3
F. @	350.28	F. @	230.07
$W_o(s^2p^2)$	7,244.72	$W_o(sp^2)$	97,694.64
$W_o(sp^3)$	114,928.50	$W_o(p^3)$	167,067.43
s.d.	3,482.04	s.d.	3,856.23
$F_2(pp)$	1,699.60	$F_2(pp)$	1,903.29
s.d.	196.43	s.d.	258.26
$G_1(sp)$	19,116.03	$G_1(sp)$	22,523.57
s.d.	1,103.45	s.d.	1,928.11
*$W_o(p^4)$	222,632.28	+*$W_o(s^2p)$	42.66

* Terms estimated using ΔW_o relationship.

+* Terms calculated by hand.

@Note:

The variance ratio F is the ratio of the estimate of variance for the improvement due to regression to the estimate of the variance of the regression itself. Thus F measures the goodness of fit and is to be compared with a critical F taken from standard tables.

The degree of freedom is expressed, in Tables 31-54, as D.F. with the number of independent variables n in the numerator and the number of degrees of freedom (= N - n-1, where n is the number of data used) in the denominator.

Table 26. Parameters for Sc I

	d^2s	d^2p	Total regression
D.F.	3/3	5/6	11/15
F.	1,667.95	2.47	26.95
$W_o(d^2s)$	18,876.09		16,544.21
$W_o(d^2p)$		36,779.85	36,053.96
s.d.			2,045.21
$W_o(d^3)$			34,063.53
s.d.			2,196.89
$W_o(dsp)$			21,832.37
s.d.			2,236.18
$W_o(dp^2)$			50,448.49
s.d.			4,009.84
$W_o(ds^2)$			101.00
$F_2(pd)$		286.72	179.47
s.d.		259.74	178.50
$F_2(dd)$	593.30	133.65	363.45
s.d.	9.75	138.40	88.19
$F_4(dd)$	32.55	-89.38	29.83
s.d.	1.43	30.96	17.97
$G_1(pd)$		298.79	104.99
s.d.		311.43	239.25
$G_3(pd)$		83.73	38.79
s.d.		45.34	35.68
$G_1(sp)$			3,023.59
s.d.			2,831.38
$G_2(sd)$	1,146.24		1,044.05
*$F_2(pp)$			483.68

* Term calculated from ΔW_o relationship.

Table 27. Parameters for Sc II

-	d^2	dp	Total regression
D.F.	2/2	3/3	12/4
F.	2,197.00	17.35	
$W_o(s^2)$			11,736.35
$W_o(ds)$			1,327.17
$W_o(p^2)$			76,396.90
$W_o(d^2)$	11,276.13		11,276.13
$W_o(sp)$			47,434.58
$W_o(pd)$		28,952.25	28,952.25
$F_x(pd)$		242.07	242.07
s.p.		49.21	49.21
$F_2(dd)$	738.71		738.71
	3.52		3.52
$F_4(dd)$	51.75		51.75
s.d.	0.47		0.47
$G_1(pd)$		382.03	382.03
s.d.		72.86	72.86
$G_3(pd)$		2.76	2.76
s.d.		7.40	7.40
$G_1(sp)$			8,280.93
$G_2(sd)$			1,214.80

Table 28. Parameters for Ti I

	d^2s^2	d^3s	d^3p	Total regression
D.F.	2/2	3/8	5/14	13/41
F.	90.40	4.65	10.46	8.4
$W_o(d^2s^2)$	7,976.16			7,413.91
$W_o(d^3s)$		20,184.79		20,682.49
s.d.				1,773.63
$W_o(d^3p)$			41,004.20	42,099.95
s.d.				1,602.15
$W_o(d^2sp)$				31,676.14
s.d.				1,802.43
$W_o(d^4)$				40,408.46
s.d.				2,846.24
$W_o(d^2p^2)$				54,333.64
s.d.				4,961.18
$F_2(pd)$			94.39	137.53
s.d.			142.51	108.51
$F_2(dd)$	916.17	296.59	211.17	411.24
s.d.	68.28	247.13	117.45	73.97
$F_4(dd)$	67.71	26.14	20.53	27.55
s.d.	9.17	24.84	24.40	12.69
$G_1(pd)$			175.35	195.46
s.d.			13.17	149.48
$G_3(pd)$			97.97	17.30
s.d.			36.71	21.18
$G_1(sp)$				4,028.73
s.d.				2,118.07
$G_2(sd)$		1,449.48		1,348.58
s.d.		937.51		690.05
$F_2(pp)$				555.91
s.d.				1,170.76

Table 29. Parameters for Ti II

	d^2s	d^3	d^2p	Total regression
D.F.	3/4	2/4	5/6	11/18
F.	18.85	66.00	6.77	242.43
$W_o(d^2s)$	10,798.96			10,913.96
$W_o(ds^2)$				25,066.34
s.d.				2,033.91
$W_o(d^3)$		16,446.64		15,736.09
s.d.				1,278.64
$W_o(d^2p)$			40,772.05	40,552.55
s.d.				1,285.45
$W_o(dsp)$				64,220.68
s.d.				1,620.78
$F_2(pd)$			435.19	368.66
s.d.			256.71	114.15
$F_2(dd)$	783.24	856.31	688.59	765.75
s.d.	114.29	74.64	193.06	58.87
$F_4(dd)$	19.73	52.85	11.63	28.76
s.d.	13.40	10.51	40.05	8.10
$G_1(pd)$			432.94	343.19
s.d.			315.28	179.67
$G_3(pd)$			41.61	25.32
s.d.			45.05	23.38
$G_1(sp)$				7,359.04
s.d.				2,182.89
$G_2(sd)$	1,693.84			1,767.85
s.d.	762.03			625.47
$*W_o(d^2p^2)$				93,859.27
$*F_2(pp)$				700.00

* Estimated values, using ΔW_o approximation.

Table 30. Parameters for V I

	d^3s^2	d^4s	d^4p	Total regression
D.F.	2/3	3/4	5/1	13/13
F.	109.47	4.12	6.08	44.50
$W_o(d^3s^2)$	21,310.34			17,403.72
$W_o(d^4s)$		33,665.18		33,235.94
s.d.				2,518.79
$W_o(d^5)$				57,798.64
s.d.				4,194.05
$W_o(d^3p^2)$				72,963.39
s.d.				5,520.68
$W_o(d^4p)$			47,123.23	45,825.96
s.d.				3,360.49
$W_o(d^3sp)$				50,100.33
s.d.				4,062.31
$F_2(pp)$				1,077.88
s.d.				1,512.40
$F_2(pd)$			-75.45	193.95
s.d.			463.34	225.17
$F_2(dd)$	1,000.36	738.78	297.57	696.37
s.d.	77.95	404.51	347.91	115.05
$F_4(dd)$	85.05	50.91	87.00	50.35
s.d.	6.86	33.84	45.93	13.74
$G_1(pd)$			-263.73	296.06
s.d.			548.95	301.62
$G_3(pd)$			4.69	-26.05
s.d.			7.98	42.24
$G_1(sp)$				14,987.98
s.d.				640.81
$G_2(sd)$		1,201.85		1,323.67
s.d.		1,168.33		833.21

Table 31. Parameters for V II

	d^4	d^3s	d^3p	Total regression
D.F.	2/8	3/7	5/14	10/34
F.	1,765.47	8.89	13.17	45.06
$W_o(d^4)$	31,372.05			26,981.05
$W_o(d^3s)$		25,150.68		24,755.59
s.d.				3,020.10
$W_o(d^2sp)$				68,374.30
s.d.				10,534.10
$W_o(d^3p)$			58,069.31	61,230.32
s.d.				7,952.90
$F_2(pd)$			295.02	298.16
s.d.			181.60	191.79
$F_2(dd)$	754.42	665.62	841.31	564.87
s.d.	18.16	180.17	170.13	126.99
$F_4(dd)$	80.98	77.45	51.83	58.58
s.d.	3.03	35.22	29.61	24.05
$G_1(pd)$			146.37	143.67
s.d.			239.47	255.78
$G_3(pd)$			40.42	192.98
s.d.			47.03	289.34
$G_1(sp)$				-6,759.06
s.d.				9,346.73
$G_2(sd)$		602.99		1,149.21
s.d.		1,458.97		1,414.26
$+W_o(d^2s^2)$				18,929.31
$*W_o(d^2p^2)$				84,766.57

* Terms estimated from ΔW_o relationship.

\+ Terms calculated separately by hand.

Table 32. Parameters for Cr I

	d^5s	d^4s^2	d^5p	Total regression
D.F.	3/12	2/6	4/11	11/40
F.	34.45	4.4	12.91	43.25
$W_o(d^5s)$	52,412.98			52,862.59
$W_o(d^4s^2)$		37,583.72		38,337.87
s.d.				2,883.91
$W_o(d^6)$				62,587.60
s.d.				5,043.89
$W_o(d^5p)$			72,963.41	70,824.06
s.d.				3,256.06
$W_o(d^4sp)$				62,604.34
s.d.				1,218.84
*$W_o(d^4p^2)$				80,565.81
$F_2(pd)$				180.23
s.d.				67.76
$F_2(dd)$	464.45	535.17	806.71	549.32
s.d.	114.06	361.40	187.39	94.99
$F_4(dd)$	88.14	74.94	70.09	82.07
s.d.	12.95	39.27	19.82	10.53
$G_1(pd)$			-848.00	-279.09
s.d.			450.86	312.55
$G_3(pd)$			17.79	-25.01
s.d.			49.41	34.11
$G_1(sp)$				9,084.58
s.d.				11,335.99
$G_2(sd)$	1,059.21			960.50
s.d.	823.53			882.49

* Term estimated by using ΔW_o approximation.

Table 33. Parameters for Cr II

	d^5	d^4s	$d^3\,{}^2$ $+d^4p$	Total regression
D.F.	2/9	3/8	5/17	9/35
F.	68.57	12.23	2.89	80.94
$W_o(d^5)$	57,365.09			51,426.82
$W_o(d^4s)$		48,690.91		47,799.51
s.d.				3,329.46
$W_o(d^3s^2)$			58,625.13	62,663.37
s.d.				2,947.17
$W_o(d^4p)$			85,990.09	83,218.94
s.d.				3,412.36
$F_2(pd)$			421.56	399.07
s.d.			232.40	394.24
$F_2(dd)$	951.32	295.23	349.53	594.94
s.d.	130.05	217.21	120.63	96.55
$F_4(dd)$	70.03	111.87	100.96	72.12
s.d.	13.71	27.04	19.62	13.47
$G_1(pd)$			527.14	194.25
s.d.			252.82	405.21
$G_3(pd)$			79.07	67.31
s.d.			33.77	44.52
$G_2(sd)$		1,732.97		1,817.31
s.d.		966.13		1,121.05
$^*W_o(d^3p^2)$				115,011.07
$^*W_o(d^3sp)$				79,591.63

* Terms obtained by using ΔW_o approximation.

Table 34. Parameters for Mn I

	d^5s^2	d^6s	d^6p	Total regression
D.F.	2/2	3/5	5/3	12/17
F.	253.18	16.73	201.25	41.61
$W_o(d^5s^2)$	74,363.58			60,877.57
$W_o(d^6s)$		49,950.56		53,457.20
s.d.				4,823.83
$W_o(d^6p)$			52,060.21	52,396.64
s.d.				2,096.25
$W_o(d^5p^2)$				94,272.73
s.d.				1,711.39
$W_o(d^5sp)$				86,000.52
s.d.				5,979.49
$F_2(pd)$			153.48	170.91
s.d.			61.30	34.97
$F_2(dd)$	1,346.99	1,107.89	544.21	554.52
s.d.	93.91	183.53	130.69	180.17
$F_4(dd)$	85.92	139.93	112.13	121.92
s.d.	7.61	28.29	13.29	20.16
$G_1(pd)$			-837.16	-851.11
s.d.			276.72	685.83
$G_3(pd)$			-15.36	-17.86
s.d.			25.92	66.95
$G_1(sp)$				8,174.91
s.d.				818.95
$G_2(sd)$		886.24		942.44
s.d.		846.10		110.54
$W_o(d^7)$				65,636.58

Table 35. Parameters for Mn II

	d^6	d^5s	d^5p	Total regression
D.F.	2/4	3/6	4/9	
F.	3.01	6.73	15.02	
$W_o(d^6)$	43,366.74			43,366.74
$W_o(d^5s)$		49,459.53		49,459.53
$W_o(d^5p)$			91,556.21	91,556.21
$W_o(d^4s^2)$				80,566.24
$W_o(d^4sp)$				134,394.82
$W_o(d^4p^2)$				176,490.68
$F_2(pd)$				325.21
$F_2(dd)$	612.26	705.25	551.11	612.26
s.d.	430.26	350.03	219.03	
$F_4(dd)$	66.22	60.06	93.95	66.22
s.d.	65.17	42.33	26.13	
$G_1(pd)$			585.21	489.00
s.d.			65.45	
$G_3(pd)$			33.71	32.00
s.d.			77.85	
$G_1(sp)$				-3,627.65
$G_2(sd)$		1,632.66		1,632.66
s.d.		200.24		

Note: The total regression was done by substitution of known parameters into equations of configurations d^4s^2, d^4sp d^4p^2.

Table 36. Parameters for Fe I

	d^6s^2	d^7s	d^7p	Total regression
F.	5,635.21	579.44	270.51	984.15
D.F.	2/2	3/8	5/4	9/20
$W_o(d^6s^2)$	51,167.58			49,379.22
$W_o(d^7s)$		31,194.53		37,632.67
s.d.				599.00
$W_o(d^7p)$			63,962.27	63,648.40
s.d.				1,553.00
$W_o(d^7sp)$				77,139.79
s.d.				2,206.00
$F_2(pd)$			146.15	179.25
s.d.			35.60	39.80
$F_2(dd)$	1,386.66	1,265.79	1,316.31	1,312.07
s.d.	18.90	31.20	53.00	26.20
$F_4(dd)$	106.87	102.81	100.45	106.87
s.d.	1.09	4.40	6.86	3.33
$G_1(pd)$			53.47	82.59
s.d.			52.30	68.60
$G_3(pd)$			7.67	-0.01
s.d.			9.63	8.23
$G_2(sd)$		1,331.39		1,331.39
s.d.		149.50		161.42
$W_o(d^8)$				44,724.07
$W_o(d^5s^2p)$				120,674.65
$*W_o(d^6p^2)$				103,155.52

* Term estimated from ΔW_o approximate relationship.

Table 37. Parameters for Fe II

	d^7	d^6s	d^6p	Total regression
D.F.	2/4	3/10	5/2	8/21
F.	452	1,567	1,574	1,099
$W_o(d^7)$	28,335.37			29,337.43
$W_o(d^6s)$		56,871.32		56,837.98
s.d.				623.00
$W_o(d^5s^2)$				108,132.68
s.d.				1,354.00
$W_o(d^6p)$			102.063.	103,967.91
s.d.				7,828.00
$F_2(pd)$			318.44	321.80
s.d.			39.80	101.90
$F_2(dd)$	1,350.38	1,261.46	1,328.23	1,350.38
s.d.	43.60	28.60	86.70	30.00
$F_4(dd)$	97.44	115.55	119.98	112.98
s.d.	6.37	3.91	12.80	4.32
$*G_1(sp)$				17,245.91*
$G_1(pd)$			252.58	219.52
s.d.			311.20	383.00
$G_3(pd)$			12.31	30.72
s.d.			28.00	17.50
$G_2(sd)$		1,637.58		1,627.43
s.d.		120.90		187.00
$W_o(d^5sp)$ $-G_1(sp)$		152,804.35		150.900.45
$*W_o(d^5p^2)$				178,598.39

* Terms obtained by using ΔW_o relationship.

Table 38. Parameters for Co I

	$d^7s^2+d^8s$	d^8p+d^8s	Total regression
D.F.	4/5	8/2	11/8
F.	35.66	9.54	30.63
$W_o(d^7s^2)$	32,235.13		33,156.49
$W_o(d^8s)$	19,919.11		21,297.90
s.d.	1,583.11		2,619.09
$W_o(d^8p)$		54,988.51	54,988.51
s.d.			2,660.21
$W_o(d^7sp)$			64,203.50
s.d.			2,103.07
$F_2(pd)$		193.29	185.57
s.d.		191.14	202.30
$F_2(dd)$	1,451.53	1,084.61	1,268.07
s.d.	126.35	232.78	222.18
$F_4(dd)$	136.42	157.21	124.99
s.d.	14.41	38.60	21.16
$G_1(pd)$		260.78	151.03
s.d.		457.84	316.49
$G_3(pd)$		117.87	74.58
s.d.		51.71	68.44
$G_1(sp)$			7,979.03
$G_2(sd)$	912.81	755.12	833.96
s.d.	620.77	1,254.35	1,213.49
$W_o(d^9)$			27,984.78
s.d.			4,265.56
$^*W_o(d^7p^2)$			81,992.23

* Term estimated from ΔW_o relationship.

Note: Values given by Racah (35):

$F_2(dd) = 1,393.00$
$F_4(dd) = 119.10$
$G_2(sd) = 1,128.00$

Table 39. Parameters for Co II

	d^8d^7s	d^7p	Total regression
D.F.	4/3	5/3	11/4
F.	5.49	7.03	48.53
$W_o(d^8)$	8,613.18		8,395.35
$W_o(d^7s)$	27,557.96		25,343.72
s.d.	4,976.64		4,431.85
$W_o(d^7p)$		48,985.06	48,985.06
$W_o(d^6sp)$			59,892.00
$F_2(pd)$		405.19	339.22
s.d.		207.60	309.18
$F_2(dd)$	855.81	654.15	754.18
s.d.	221.19	250.19	174.89
$F_4(dd)$	24.51	18.76	29.46
s.d.	35.36	45.42	29.46
$G_1(pd)$		-1,416.00	-1,327.42
s.d.		526.27	
$G_3(pd)$		-154.90	-194.81
s.d.		145.23	
$G_1(sp)$			15,187.06
$G_2(sd)$	1,342.95		1,331.45
s.d.	1,316.86		1,172.44
$W_o(d^6s^2)$			63,952.26
s.d.			8,525.99
*$W_o(d^6p^2)$			86,555.05

* Term estimated from ΔW_o relationship.

Table 40. Parameters for Ni I

	d^9p	$d^8s^2+d^8sp$	Total regression
D.F.	3/2	7/3	10/5
F.	5.13	218.83	106.15
$W_o(d^9p)$	31,992.94		32,079.22
s.d.			1,543.73
$W_o(d^8s^2)$		14,764.25	14,943.90
s.d.			1,185.64
$W_o(d^8sp)$		54,614.89	56,595.44
s.d.			10,830.72
$F_2(pd)$	107.58	107.58	132.22
s.d.	62.08	72.19	189.43
$F_2(dd)$		1,632.81	1,630.54
s.d.		92.71	1,143.19
$F_4(dd)$		120.61	133.51
s.d.		12.45	16.91
$G_1(pd)$	189.99	189.99	221.17
s.d.	48.98	56.96	121.84
$G_3(pd)$	14.56	14.56	20.12
s.d.	9.54	11.09	20.57
$G_1(sp)$			2,193.23
s.d.			2,815.91
$G_2(sd)$			1,364.41
s.d.			984.57
$W_o(d^{10})$			14,728.85
$W_o(d^9s)$			2,045.05
*$W_o(d^8p^2)$			98,246.98

* Term calculated from ΔW_o approximate relationship.

Table 41. Parameters for Ni II

	d^8s	d^8p	Total regression
D.F.	3/2	6/4	8/4
F.	142.00	13.00	138.75
$W_o(d^8s)$	26,477.23		24,961.96
$W_o(d^8p)$		81,201.44	74,264.48
s.d.			6,551.29
$F_2(dd)$	1,637.36	1,012.38	1,297.78
s.d.	82.46	200.37	164.56
$F_4(dd)$	117.85	-0.27	66.20
s.d.	12.09	41.57	28.39
$F_2(pd)$		260.73	312.13
s.d.		143.54	149.49
$G_1(pd)$		78.24	136.74
s.d.		340.85	355.34
$G_3(pd)$		137.22	78.81
s.d.		55.69	52.22
$G_2(sd)$	1,528.83		1,264.77
s.d.	318.99		070.86
$W_o(d^9)$			602.76
$*W_o(d^7sp)$			98,020.92
$*W_o(d^7s^2)$			49,321.16
$*W_o(d^7p^2)$			147,926.20

* Terms estimated from ΔW_o relationship.

Table 42. Parameters for Cu I

$W_o(d^{10}s)$	0.00
$W_o(d^9s^2)$	12,019.70
$W_o(d^{10}p)$	30,700.89
$W_o(d^9sp)$	66,236.99
$F_2(pd)$	315.50
$+F_2(dd)$	1,810.00
$+F_4(dd)$	148.00
$G_1(pd)$	390.62
$G_3(pd)$	6.83
$G_1(sp)$	6,906.00
$G_2(sd)$	901.00
$*W_o(d^9p^2)$	108,695.00

Note: All values are obtained by exact Solution of Matrix, except:
+ Terms obtained by extrapolation with the corresponding terms of FeI, CoI, NiI.
*Term estimated from ΔW_o relationship.

Table 43. Parameters for Cu II

	d^9s+d^9p	$d^8s^2+d^9p$	Total regression
D.F.	3/2	6/2	10/7
F.	11.16	119.06	833.22
$W_o(dp^9)$	73,749.10	73,749.10	72,097.76
s.d.			1,580.50
$W_o(d^8s^2)$		87,018.12	86,953.00
s.d.		1,049.46	1,325.59
$W_o(d^8sp)$			134,435.00
s.d.			3,902.08
$F_2(pd)$	378.93	378.93	377.57
s.d.	79.71	89.26	106.12
$F_2(dd)$		1,899.14	1,748.43
s.d.		114.65	117.80
$F_4(dd)$		135.65	130.99
s.d.		15.40	18.01
$G_1(pd)$	325.19	325.19	104.63
s.d.	62.89	70.43	104.53
$G_3(pd)$	32.59	32.59	12.76
s.d.	12.26	13.72	20.01
$G_1(sp)$			341.12
s.d.			912.34
$G_2(sd)$	1,842.25		1,231.97
s.d.			827.37
$W_o(d^{10})$			0.00
$W_o(d^9s)$	24,422.27		24,422.27
$*W_o(d^8p^2)$			181,917.00

* Term estimated from ΔW_o relationship.

Table 44. Parameters for Zn I and II

Zn I		Zn II	
$W_o(s^2)$	0.00	$W_o(s)$	0.00
$W_o(sp)$	39,671.00	$W_o(p)$	48,917.50
$W_o(p^2)$	80,710.09		
$F_2(pp)$	84.92		
$G_1(sp)$	7.073.85		

Table 45. Parameters for Ga I and II

Ga I		Ga II	
D. F.	3/1		
F.	4,003.98		
$W_o(s^2p)$	413.12	$W_o(s^2)$	0.00
$W_o sp^2)$ s.d.	61,694.75 563.69	$W_o(sp)$	59,339.35
$F_2(pp)$ s.d.	963.90 48.54	$F_2(pp)$	66.49
$G_1(sp)$ s.d.	9,233.77 275.24	$G_1(sp)$	11,360.85
*$W_o(p^3)$	122,976.38	*$W_o(p^2)$	118,678.70

*Term obtained by using ΔW_o approximation.

Table 46. Parameters for Ge I and II

Ge I		Ge II	
D.F.	3/3	D.F.	4/1
F.	73.86	F.	24.40
$W_o(s^2p^2)$	6,368.14	$W_o(s^2p)$	1,178.06
$W_o(sp^3)$	51,921.11	$W_o(sp^2)$	83,617.97
s.d.	4,379.38		
*$W_o(p^4)$	96,974.05	$W_o(p^3)$	156,014.04
		s.d.	12,452.98
$F_2(pp)$	668.93	$F_2(pp)$	1,316.05
s.d.	357.58	s.d.	617.79
$G_1(sp)$	-802.70	$G_1(sp)$	13,439.71
		s.d.	3,480.35

* Terms evaluated by using ΔW_o relationship.

Table 47. Parameters for As I and II

As I		As II	
D.F.	3/4	D.F.	3/3
$W_o(s^2p^3)$	18,416.80	F.	2,052.62
$W_o(sp^4)$	70,873.55	$W_o(s^2p^2$	8,494.26
$F_2(pp)$	1,233.28	$W_o(sp^3)$	83,099.00
		s.d.	1,286.11
$G_1(sp)$	2,483.21	$F_2(pp)$	1,456.41
		s.d.	95.86
*$W_o(p^5)$	123,330.30	$G_1(sp)$	-305.28
		s.d.	689.60
		*$W_o(p^4)$	157,703.74

* Terms estimated from ΔW_o approximation.

Table 48. Parameters for Se I and II

Se I		Se II	
$W_o(s^2p^4)$	8,156.56	D.F.	3/2
+$W_o(sp^5)$	83,323.05	F.	11,350.06
$F_2(pp)$	1,419.52	$W_o(s^2p^3)$	23,228.27
$G_1(sp)$	---	$W_o(sp^4)$	108,090.80
		s.d.	571.52
*$W_o(p^6)$	158,489.54	$F_2(pp)$	1,559.14
		s.d.	45.76
		$G_1(sp)$	5,141.32
		s.d.	230.31
		*$W_o(p^5)$	192,953.33

+ Term estimated by linear extrapolation from the corresponding terms of isoelectronic elements Br II and Kr III

* Terms calculated from ΔW_o relationship.

Table 49. Parameters for Br I and II

Br I		Br II	
$W_o(s^2p^5)$	1,228.33	$W_o(s^2p^4)$	9,798.75
+$W_o(sp^6)$	90,000.00	$W_o(sp^5)$	97,228.71
=$F_2(pp)$	1,571.39	$F_2(pp)$	1,610.25
$G_1(sp)$	---	$G_1(sp)$	---
		*$W_o(p^6)$	184,658.67

* Term calculated from ΔW_o relationship.

+ Term estimated by extrapolation from the corresponding term of isoelectronic elements Kr II, Rb III, Sr IV, Y V.

= Term obtained by linear extrapolation with $F_2(pp)$ of Se I, As I, Ge I and Ga I.

Table 50. Hybrids Orbitals Used.

Divalent	Symbols	Wave functions
	$(sp)^2$	$\begin{cases} di_1 = 1/\sqrt{2}\,(s + z) \\ di_2 = 1/\sqrt{2}\,(s - z) \end{cases}$
	$(sd)^2$	$\psi_{1,2} = \frac{1}{\sqrt{2}}(s \pm \delta)$
	$(pd)^2$	$\psi_{1,2} = \frac{1}{\sqrt{2}}(z \pm \sigma)$
	$(dd^1)^2$	$\begin{cases} \psi_1 = \frac{1}{\sqrt{3}}\sigma + \sqrt{\frac{2}{3}}\delta \\ \psi_2 = \sqrt{\frac{2}{3}}\sigma - \sqrt{\frac{1}{3}}\delta \end{cases}$ or $\begin{cases} \sqrt{\frac{1}{3}}\pi + \sqrt{\frac{2}{3}}\delta \\ \sqrt{\frac{2}{3}}\pi + \sqrt{\frac{1}{3}}\delta \end{cases}$
Trivalent	$(sp^2)^3$	$\begin{cases} \psi_1 = \sqrt{\frac{1}{3}}s + \sqrt{\frac{2}{3}}x \\ \psi_{2,3} = \sqrt{\frac{1}{3}}s - \sqrt{\frac{1}{6}}x \pm \sqrt{\frac{1}{2}}y \end{cases}$
	$(sd^2)^3$	$\begin{cases} \psi_1 = \sqrt{\frac{1}{3}}s + \sqrt{\frac{2}{3}}\pi \\ \psi_{2,3} = \sqrt{\frac{1}{3}}s - \sqrt{\frac{1}{6}}\pi \pm \sqrt{\frac{1}{2}}\pi' \end{cases}$
	$(pd^2)^3$	$\begin{cases} \psi_1 = \sqrt{\frac{1}{3}}x + \sqrt{\frac{2}{3}}\sigma \\ \psi_{2,3} = \sqrt{\frac{1}{3}}x - \sqrt{\frac{1}{6}}\sigma + \sqrt{\frac{1}{2}}\delta \end{cases}$
	(d^3)	$\begin{cases} \psi_1 = \sqrt{\frac{1}{3}}\sigma + \sqrt{\frac{2}{3}}\delta \\ \psi_{1,2} = \sqrt{\frac{1}{3}}\sigma - \sqrt{\frac{1}{6}}\delta + \sqrt{\frac{1}{2}}\delta' \end{cases}$

Table 50 (continued)

	(spd)^3	$\begin{cases}\psi_{1,2} = \sqrt{\frac{1}{12}s} \pm \sqrt{\frac{1}{2}}\,z + \sqrt{\frac{5}{12}}\,\sigma \\ \psi_3 = \sqrt{\frac{5}{6}s} - \sqrt{\frac{1}{6}}\,\sigma\end{cases}$
Tetravalent	(sp^3)^4	$\begin{cases}\psi_{1,2} = \frac{1}{2}(s + x \pm y \pm z) \\ \psi_{3,4} = \frac{1}{2}(s - x \pm y \mp z)\end{cases}$
	(dsp^2)^4	$\begin{cases}\psi_{1,2} = \frac{1}{2}s \pm \sqrt{\frac{1}{2}x} + \frac{1}{2}\delta' \\ \psi_{3,4} = \frac{1}{2}s \pm \sqrt{\frac{1}{2}y} - \frac{1}{2}\delta'\end{cases}$
	(sd^3)^4	$\begin{cases}\psi_{1,2} = \frac{1}{2}s \pm \sqrt{\frac{1}{2}\pi} + \frac{1}{2}\delta \\ \psi_{3,4} = \frac{1}{2}s \pm \sqrt{\frac{1}{2}\pi'} - \frac{1}{2}\delta\end{cases}$
	(d^4)^4	$\begin{cases}\psi_{1,2} = -\frac{1}{2}\sigma + \frac{1}{2}\delta + \sqrt{\frac{1}{2}\pi} \\ \psi_{3,4} = -\frac{1}{2}\sigma - \frac{1}{2}\delta \pm \sqrt{\frac{1}{2}\pi'}\end{cases}$
Hexavalent	(d^{2}sp^3)^6	$\begin{cases}\psi_{1,2} = \sqrt{\frac{1}{6}s} \pm \frac{1}{\sqrt{2}}z + \frac{1}{\sqrt{3}}\sigma \\ \psi_{3,4} = \sqrt{\frac{1}{6}s} \pm \frac{1}{\sqrt{2}}x + \sqrt{\frac{1}{12}}\,\sigma + \frac{1}{2}\delta \\ \psi_{5,6} = \sqrt{\frac{1}{6}s} \pm \frac{1}{\sqrt{2}}y + \frac{1}{\sqrt{12}}\sigma - \frac{1}{2}\delta\end{cases}$

Table 51. Valence State ionization potential of Sc.

No	Valence state	P.E.ScI	P.E.Sc II	V.S.I.P.
1	$V_3(s)d(sp)^2$	1.716	1.853	6.697
2	$V_3(2)d''sd)^2$	1.773	0.613	5.400
3	$V_3(2)d(pd)^2$	4.222	2.486	4.824
4	$V_3(2)s(pd)^2$	1.817	1.777	6.520
5	$V_3(2)d(dd')^2$	3.874	1.460	4.146
6	$V_3(2)s(dd')^2$	1.747	0.239	5.502
7	$V_3(3)(sp^2)^3$	2.998	5.319	8.881
8	$V_3(3)(d^2s)^3$	2.231	0.844	5.173
9	$V_3(spd)^3$	1.621	1.931	6.870
10	$V_3(pd^2)^3$	4.248	2.999	5.311
11	$V_3(d^3)^3$	4.063	1.036	3.533

Table 52. Valence state ionization potentials of Ti.

I.P. = 6.830 volts

No	Valence states	P.E.Ti I	P.E.Ti II	V.S.I.P.
1	$V_4(2)d^2(sp)^2$	1.957	2.412	7.285
2	$V_4(2)d^2(sd)^2$	1.581	1.343	6.592
3	$V_4(2)d^2(pd)^2$	4.500	3.010	5.340
4	$V_4(2)sd(pd)^2$	2.136	3.291	7.985
5	$V_2s^2(pd)^2$	0.875	5.804	11.759
6	$V_4(2)d^2(dd')^2$	3.591	1.601	4.840
7	$V_4(2)sd(dd')^2$	1.356	1.149	6.623
8	$V_2s^2(dd')^2$	0.358	2.923	9.395
9	$V_4(3)d(sp^2)^3$	3.806	7.449	10.473
10	$V_4(3)d(sd^2)^3$	1.795	0.898	5.933
11	$V_4(3)d(spd)^3$	2.221	3.433	8.042
12	$V_4(3)d(pd^2)^3$	4.640	3.820	6.010
13	$V_4(3)s(pd^2)^3$	2.299	4.706	9.239
14	$V_4(3)d(d^3)^3$	3.906	1.231	4.155
15	$V_4(3)s(d^3)^3$	1.719	0.887	5.998
16	$V_4(sp^3)^4$	6.722	13.323	13.431
17	$V_4(sd^3)^4$	1.720	1.030	6.140
18	$V_4(dsp^2)^4$	4.079	9.273	12.024
19	$V_4(d^4)^4$	3.906	1.199	4.123

Table 53. Valence state ionization potentials of V.

I.P. = 6.74 volts

No	Valence States	P.E.V I	P.E.V II	V.S.I.P.
1	$V_5(2)d^3(sp)^2$	-0.395	3.079	10.214
2	$V_5(2)d^3(sd)^2$	1.444	2.243	6.539
3	$V_5(2)d^3(pd)^2$	3.908	3.176	6.008
4	$V_5(2)sd^2(pd)^2$	0.628	5.426	11.574
5	$V_3(2)s^2d(pd)^2$	-1.121	7.553	15.414
6	$V_5(2)d^3(dd')^2$	2.890	1.263	5.113
7	$V_5(2)sd^2(dd')^2$	1.074	1.428	7.094
8	$V_3(2)s^2d(dd')$	0.305	1.644	8.079
9	$V_5(3)d^2(sp^2)^3$	2.394	9.191	13.537
10	$V_5(3)d^2(sd^2)^3$	1.842	1.514	6.412
11	$V_5(3)d^2(spd)^3$	0.715	5.283	11.308
12	$V_5(3)d^2(pd^2)^3$	4.540	4.473	6.673
13	$V_5(3)sd(pd^2)^3$	1.150	7.271	12.861
14	$V_3s^2(pd^2)^3$	0.989	9.619	15.370
15	$V_5(3)d^2(d^3)^3$	3.766	1.641	4.615
16	$V_5(3)sd(d^3)^3$	1.786	1.837	7.000
17	$V_3s^2(d^3)^3$	0.634	1.695	7.801
18	$V_5(4)d(sp^3)^4$	9.380	16.373	13.733
19	$V_5(4)d(sd^3)^4$	2.055	1.934	6.619
20	$V_5(4)d(dsp^2)^4$	3.420	11.380	14.700
21	$V_5(4)d(d^4)^4$	3.958	1.846	4.628
22	$V_5(4)s(d^4)^4$	1.868	1.882	6.754

Table 54. Valence state ionization potentials of Cr.

I.P. = 6.763 volts

No	Valence states	P.E.Cr. I	P.E.Cr II	V.S.I.P.
1	$V_6(2)d^4(sp)^2$	1.392	4.359	9.930
2	$V_6(2)d^4(sd)^2$	1.691	1.992	7.064
3	$V_6(2)d^4(pd)^2$	4.796	4.115	6.082
4	$V_6(2)sd^3(pd)^2$	2.460	3.736	8.039
5	$V_4(2)d^2d^2(pd)^2$	1.656	5.967	11.051
6	$V_4(2)d^4(dd')^2$	5.000	3.690	5.453
7	$V_6(2)sd^3(dd')^2$	1.227	2.467	8.003
8	$V_4(2)s^2d^2(dd')$	1.518	5.800	11.045
9	$V_6(3)d^3(sp^2)^3$	4.076	7.672	10.359
10	$V_6(3)d^3(sd^2)^3$	2.386	2.800	7.177
11	$V_6(3)d^3(dsp)^3$	2.638	4.297	8.422
12	$V_6(3)d^3(pd^2)^3$	5.541	5.494	6.716
13	$V_6(3)sd^2(pd^2)^3$	3.061	4.651	8.354
14	$V_4(3)s^2d(pd^2)^3$	1.993	6.121	10.891
15	$V_4(3)d^3(d^3)^3$	5.603	3.857	5.017
16	$V_6(3)sd^2(d^3)^3$	2.340	2.967	7.390
17	$V_4(3)s^2d(d^3)^3$	2.131	6.063	10.695
18	$V_6(4)d^2(sp^3)^4$	8.532	10.448	8.679
19	$V_6(4)d^2(sd^3)^4$	2.788	3.244	7.219
20	$V_6(4)d^2(dsp^2)^4$	5.112	8.076	9.727
21	$V_4(4)d^2(d^4)^4$	5.602	3.869	5.030
22	$V_6(4)sd(d^4)^4$	2.602	3.280	7.441
23	$V_4(4)s^2(d^4)^4$	2.121	6.051	10.693

Table 55. Valence state ionisation potentials of Mn.

I.P. = 7.432 volts

No	Valence States	P.E.Mn I	P.E.Mn II	V.S.I.P.
1	$V_7(2)d^5(sp)^2$	1.051	3.464	9.845
2	$V_5(2)d^5(sd)^2$	3.174	3.084	7.342
3	$V_5(2)d^5(pd)^2$	6.071	3.853	5.214
4	$V_7(2)sd^4(pd)^2$	2.878	7.744	12.298
5	$V_5(2)s^2d^3(pd)^2$	4.423	16.871	19.880
6	$V_3(2)d^5(dd')^2$	6.467	4.507	5.472
7	$V_5(2)sd^4(dd')^2$	1.520	4.789	10.701
8	$V_5(2)s^2d^3(dd')^2$	0.819	7.906	14.519
9	$V_7(3)d^4(sp^2)^3$	5.849	14.603	16.186
10	$V_5(3)d^4(sd^2)^3$	3.792	4.014	7.654
11	$V_7(3)d^4(spd)^3$	3.030	7.161	11.563
12	$V_7(3)sd^3(pd^2)^3$	3.802	11.288	14.918
13	$V_5(3)d^4(pd^2)^3$	6.722	5.749	6.459
14	$V_5(3)s^2d^2(pd^2)^2$	5.085	21.416	23.763
15	$V_3d^4(d^3)^3$	6.762	4.217	4.887
16	$V_5(3)sd^3(d^3)^3$	3.570	4.066	7.928
17	$V_5(3)s^2d^2(d^3)^3$	2.101	8.280	13.611
18	$V_7(4)d^3(te)^4$	13.253	34.897	29.076
19	$V_5(4)d^3(sd^3)^4$	4.106	4.410	7.736
20	$V_7(4)d^3(dsp^2)^4$	7.536	19.706	19.602
21	$V_5(4)s^2d(d^4)^4$	2.355	8.476	13.553
22	$V_5(4)sd^2(d^4)^4$	3.628	4.017	7.821

Table 56. Valence state ionization potentials of Fe.

I.P. = 7.896 volts

No	Valence states	P.E.Fe I	P.E.Fe II	V.S.I.P.
1	$V_4(2)d^4s^2(dd')^2$	1.283	6.428	12.978
2	$V_4(2)d^6(sd)^2$	2.168	2.207	7.939
3	$V_2d^5(dd')^2(dd')^+$	5.030	3.733	6.602
4	$V_6(2)d^6(sp)^2$	3.298	2.870	7.472
5	$V_6(2)sd^5(pd)$	4.644	6.345	9.601
6	$V_6(2)d^5(spd)+(spd)^2$	4.602	5.882	9.180
7	$V_4(2)d^6(pd)^2$	9.688	7.478	5.690
8	$V_4(3)s^2d^3(d^3)^3$	2.316	7.585	13.169
9	$V_4(3)d^5(sd^2)^3$	2.916	3.764	8.748
10	$V_6(3)d^5(spd)^3$	4.997	7.793	10.196
11	$V_4(4)s^2d^2(d^4)^4$	2.316	7.626	13.210
12	$V_4d^4(sd^3)^4$	2.740	3.525	8.685

Table 57. Valence state ionization potentials of Co.

I.P. = 7.86 volts

No	Valence states	P.E. Co I	P.E. Co II	V.S.I.P.
1	$V_3(2)d^7(sd)^2$	1.825	1.501	7.536
2	$V_5(2)d^7(di)^2$	3.699	6.240	10.401
3	$V_3(2)d^7(pd)^2$	4.961	5.792	9.171
4	$V_5(2)sd^6(pd)^2$	4.636	5.290	9.126
5	$V_7(3)d^6tr^3$	8.190	8.672	8.342
6	$V_3d^6(sd^2)^3$	2.166	2.301	7.995
7	$V_3d^6(pd^2)^3$	5.051	7.569	10.378
8	$V_5(3)sd^5(pd^2)^3$	5.168	6.662	9.354
9	$V_5(d)d^6(spd)^3$	4.921	5.713	8.652
10	$V_7(4)d^5(dsp^2)^4$	9.659	7.801	6.002
11	$V_9(4)d^5te^4$	14.228	2.564	-3.802

Table 58. Valence state ionization potentials of Ni.

I.P. = 7.633 volts

No	Valence states	P.E.Ni I	P.E.Ni II	V.S.I.P.
1	$V_2d^8(sd)^2$	0.756	1.975	8.952
2	$V_4(2)d^8di^2$	3.972	4.083	7.744
3	$V_2d^8(pd)^2$	4.505	4.403	7.531
4	$V_4(2)sd^7(pd)^2$	5.135	5.276	7.774
5	$V_2s^2d^6(dd')^2$	0.615	5.097	12.115
6	$V_6(3)d^7tr^3$	13.130	9.238	3.741
7	$V_4(3)pd^6(sd^2)^3$	5.310	8.630	10.953
8	$V_4(3)sd^6(pd^2)^3$	5.539	6.543	8.637
9	$V_4(3)d^7(spd)^3$	5.305	5.228	7.556
10	$V_6(4)d^6(dsp^2)^4$	15.123	11.181	3.691
11	$V_8(4)d^6te^4$	27.780	15.214	-4.933

Table 59. Valence state ionization potentials of Cu.

I.P. = 7.723 volts

No	Valence states	P.E. Cu I	P.E. Cu II	V.S.I.P.
1	$V_1 d^{10} di$	1.903	0.000	5.821
2	$V_1 d^8 p^2 (sd)$	17.086	23.065	13.703
3	$V_1 d^8 s^2 (pd)$	5.988	12.229	13.965
4	$V_3 (2) d^8 p (sd)^2$	5.933	12.893	14.684
5	$V_3 (2) d^9 di^2$	5.679	5.776	7.821
6	$V_3 (2) d^8 s (pd)^2$	6.542	10.068	11.250
7	$V_5 (3) d^8 tr^3$	16.652	16.282	7.354
8	$V_3 d^6 s^2 (pd^2)^3$	9.104	21.482	20.102
9	$V_3 (3) d^8 (spd)^3$	6.527	9.545	10.742

Table 60. Valence state ionization potentials of X = Zn, Ga, Ge, As, Se, Br.

Element	Valence States	P.E.X I	P.E.X II	V.S.I.P.
Zn	$V_2\underline{di}^2$	4.067	3.032	8.356
Ga	$V_3\underline{tr}^3$	5.401	9.017	9.616
Ge	$V_4\underline{te}^4$	5.814	10.134	12.200
As	$V_3p^2\underline{tr}^3$	6.136	12.291	16.155
	$V_3te^2(\underline{te})^3$	4.760	9.266	14.506
Se	$V_2p^4\underline{di}^2$	6.897	15.476	18.329
	$V_2p^2tr^2\underline{tr}_1\underline{tr}_2$	4.124	11.054	16.680
	$V_2te'^2, te''^2, \underline{te'''}\underline{te''''}$	2.744	8.855	15.861
Br	$V(1)te'^2te''^2 te'''^2, \underline{te''''}$	-1.479	4.088	17.407
	$V(1)p^2tr'^2tr''^2 \underline{tr'''}$	-0.725	5.467	18.032
	$V(1)p^4s^2\ \underline{p}$	-3.743	-1.480	14.103
	$V(1)p^4di'^2\underline{di''}$	0.785	8.259	19.314

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Unclassified Report

Slater parameters (F's and G's) were calculated for the elements scandium to bromine and are tabulated. These parameters were used to calculate the energies of a wide variety of valence states of these elements, and of their unipositive ions, and hence valence state ionization potentials are derived. These data are tabulated.

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DEPARTMENT OF THE AIR FORCE
AIR FORCE RESEARCH LABORATORY
WRIGHT-PATTERSON AIR FORCE BASE OHIO 45433

December 12, 2016

MEMORANDUM FOR AFRL/RXOP
ATTN: Robin Hayes

FROM: AFRL/RXAS

SUBJECT: Technical reports WADD-TR-61-84-PT-1 and WADD-TR-61-84-PT-2

I have read through both technical reports you sent me - reference WADD-TR-61-84-PT-1 (U) Empirical Methods for Calculation of Bond Energies. Part 1 dated May 1961 and WADD-TR-61-84-PT-2 (U) Empirical Methods for Calculation of Bond Energies. Part 2 dated Sep 1963. In both cases the computations that were done, while significant in the early 1960s, could be reproduced now with better accuracy by modern computational methods and equipment in a matter of a few hours. Thus the data presented in the reports is of historical value only. Since I saw no discussions of specific strategic materials or weapon systems, I conclude that both reports should be assigned a distribution statement A. If you have any further questions, please feel free to contact me by e-mail at alan.yeates@us.af.mil or by phone at 312-785-9138 or (937)255-9138 (comm).

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