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LAFON, Earl Edward, 1940-
ENERGY BAND STRUCTURE OF LITHIUM BY THE TIGHT-BINDING METHOD.

The University of Oklahoma, Ph.D., 1967
Physics, solid state

University Microfilms, Inc., Ann Arbor, Michigan

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UNIVERSITY OF OKLAHOMA

GRADUATE COLLEGE

ENERGY BAND STRUCTURE OF LITHIUM BY THE TIGHT-BINDING METHOD

A DISSERTATION

SUBMITTED TO THE GRADUATE FACULTY

in partial fulfillment of the requirements for the

degree of

DOCTOR OF PHILOSOPHY

BY

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1967

ENERGY BAND STRUCTURE OF LITHIUM BY THE TIGHT-BINDING METHOD

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ACKNOWLEDGEMENT

The author wishes to express his sincere appreciation to Professor Chun C. Lin for his constant guidance and invaluable advice.

The author also wishes to thank his wife, Barbra, for her invaluable aid in numerical analysis and computer programming as well as for her constant cheerfulness and encouragement.

I would also like to express my most sincere appreciation to H. B. Gibbons, D. D. Eden, E. M. Wilkins, and K. G. Sewell of the Ling-Temco-Vaught Research Center for their continual interest and for making their computer facilities available.

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CHAPTER I

PRELIMINARY CONSIDERATIONS

The crystalline structure of lithium is body-centered cubic with fundamental lattice constant $a_0 = 6.5183$ au. To visualize this structure, consider any atom in the crystal and choose the origin to coincide with this atom. Next consider the set of nearest neighbors to the origin. For a body-centered cubic there are eight nearest neighbors and these eight atoms are so situated as to lie at the eight corners of a cube of side a_0 centered about the origin--thus the term body-centered cubic. The following sections describe some of the terminology and techniques useful in dealing with such periodic structures.

A. The Crystal Lattice and the Primitive Unit Cell.

The translational periodicity of any crystalline structure can be uniquely defined by the three vectors $\vec{a}_1$, $\vec{a}_2$, and $\vec{a}_3$ called the basic primitive translations. Rigid translation of the crystal by $\vec{a}_1$, $\vec{a}_2$, or $\vec{a}_3$ leaves the crystal unchanged. Thus any rigid translation by

$$\vec{R}_{\vec{n}} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3 \qquad (1)$$

where n_1, n_2, n_3 are integers is also a symmetry translation. The set of vectors $\vec{R}_{\vec{n}}$ are called the primitive translations of the crystal and the parallelopiped defined by $\vec{a}_1$, $\vec{a}_2$, and $\vec{a}_3$ is called the primitive unit cell. From these considerations it follows that any function which is periodic with the periodicity of the crystal is uniquely defined by the basic primitive translations $\vec{a}_1$, $\vec{a}_2$, $\vec{a}_3$ and by giving the value of the function at every point in the primitive unit cell.

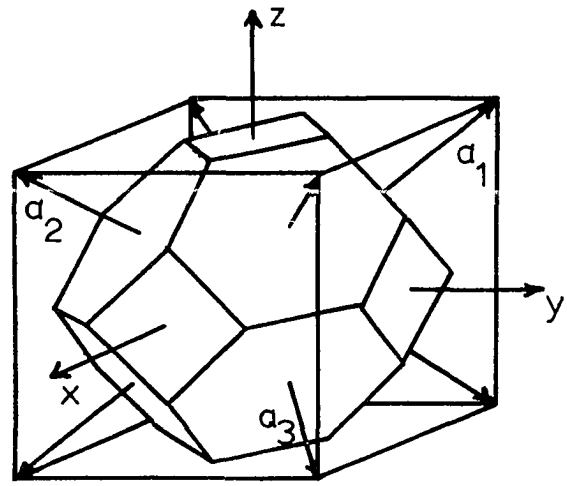
B. The Wigner-Seitz Unit Cell.

The Wigner-Seitz cell is an alternative choice for the unit cell of the lattice generated by $\vec{R}_{\vec{n}}$ and has the advantage of displaying the rotational symmetry of the crystal more clearly than does the primitive unit cell. For any of the fourteen Bravais lattices, of which the body-centered cubic is a member, the Wigner-Seitz unit cell is defined as the collection of all points in space which are closer to the lattice site situated at the origin than they are to any other lattice site in the crystal. The Wigner-Seitz unit cell for a body-centered cubic lattice is given in Fig. 1. Again, just as in the case of the primitive unit cell, any function $f(\vec{r})$ which is periodic with the periodicity of the crystal is uniquely defined by the basic primitive translations $\vec{a}_1$, $\vec{a}_2$, $\vec{a}_3$ and by giving the value of $f(\vec{r})$ at every point in the Wigner-Seitz unit cell.

C. Fourier Series.

Such a periodic function $f(\vec{r})$ as that described above can be represented by a Fourier series of the form

I) Body-Centered Cubic Crystal Lattice Cell



II) Reciprocal Lattice Cell for Body-Centered Cubic Crystal Lattice

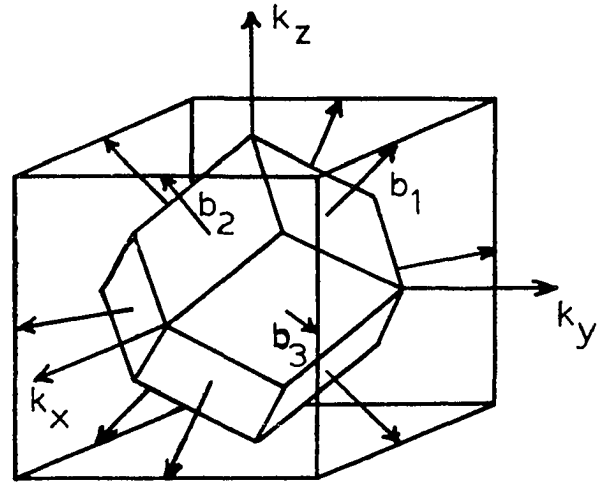


Figure 1. -- Wigner-Seitz Cells.

$$f(\vec{r}) = \sum_{\vec{K}_{\vec{m}}} f_{\vec{K}_{\vec{m}}} e^{i\vec{K}_{\vec{m}}\cdot\vec{r}} . \tag{2}$$

The periodicity of the function $f(\vec{r})$ leads to the requirement

$$f(\vec{r} + \vec{R}_{\vec{n}}) = f(\vec{r}) , \tag{3}$$

where $\vec{R}_{\vec{n}}$ is given by Eq. (1). The substitution of Eq. (2) into Eq. (3) yields the requirement

$$\vec{K}_{\vec{m}} \cdot \vec{a}_i = 2\pi m_i ; \; i = 1,2,3, \tag{4}$$

where the m_i are integers. Eq. (4) uniquely determines the allowed values of $\vec{K}_{\vec{m}}$. These are given by

$$\vec{K}_{\vec{m}} = m_1\vec{b}_1 + m_2\vec{b}_2 + m_3\vec{b}_3 , \tag{5}$$

where the m_i are integers and where

$$\vec{b}_i \cdot \vec{a}_i = 2\pi\delta_{ij} . \tag{6}$$

The symbol δ_{ij} denotes the Kronecker delta defined in the usual manner. This yields

$$\begin{aligned} \vec{b}_1 &= \frac{2\pi\vec{a}_2 \times \vec{a}_3}{[a_1a_2a_3]} , \\ \vec{b}_2 &= \frac{2\pi\vec{a}_3 \times \vec{a}_1}{[a_1a_2a_3]} , \\ \vec{b}_3 &= \frac{2\pi\vec{a}_1 \times \vec{a}_2}{[a_1a_2a_3]} , \end{aligned} \tag{7}$$

and the Fourier coefficients are given by

$$\vec{f}_{\vec{K}_{\vec{m}}} = \frac{1}{\Omega} \int_{\Omega} f(\vec{r}) \; e^{-i\vec{K}_{\vec{m}}\cdot\vec{r}} \, d\tau , \tag{8}$$

where Ω is the volume of the unit cell.

The vectors $\vec{b}_1, \vec{b}_2$, and $\vec{b}_3$ are called the basic primitive translations

of the reciprocal lattice generated by the $\vec{K}_m$ and the parallelopiped formed from $\vec{b}_1$, $\vec{b}_2$, and $\vec{b}_3$ is called the primitive unit cell of the reciprocal lattice. For a body-centered cubic crystal such as lithium, the primitive translations $\vec{K}_m$ generate a face-centered cubic structure in reciprocal space. The Wigner-Seitz cell of this reciprocal lattice is shown in Figure 1.

D. Atomic Units.

Hartree atomic units are used throughout this paper. Unless otherwise designated, all numbers which appear here are understood to be in this set of units. Hartree atomic units are characterized by

(1) Unit of mass ≡ rest mass of electron,

(2) Unit of charge ≡ magnitude of charge on the electron,

(3) Unit of length ≡ radius of first Bohr orbit of the hydrogen atom,

(4) Unit of energy ≡ twice the ionization energy of the normal state of the atom.

E. Energy Band Calculations.

At the present time there exists a large number of different methods for calculating the energy bands of crystalline solids. The most widely used of these are the methods of Orthogonalized Plane Waves (OPW), Augmented Plane Waves (APW) and Green's Function (GF). Applications of the method of tight-binding have hitherto been mostly of a qualitative or semi-empirical nature. The immense difficulties connected with the evaluation of the multicenter integrals

involved in a tight-binding application have previously made it necessary to introduce certain rather severe approximations. For example, one of the most common approximations is to ignore all multicenter integrals except those which involve nearest neighbors, [1] or next nearest neighbors. [2] In some cases these integrals are treated as parameters using an interpolative scheme, [3] while in others they are evaluated directly. [4] It is also a common practice to omit all three-center integrals from consideration. [5] While the approximation of neglecting all integrals except nearest or next nearest neighbors is applicable for core states and the d-bands of some transition metals where overlap between neighboring orbitals is small, [2] it is not valid for the general case as is demonstrated by Nran' yan [6] for diamond and by Corbato [7] for graphite. Thus, only qualitative results can be expected if this approximation were to be used in tight-binding calculations for crystals where there exists a substantial long range overlap between neighboring orbitals. Indeed, the lack of quantitative success has aroused the suspicion that the method of tight-binding is incapable of providing more than a qualitative picture for crystals with strong overlap. [8]

The recent developments of the technique of numerical integration have made it possible to evaluate the multicenter integrals arising in molecular and solid-state problems by means of electronic computers. With these new devices detailed calculations of the band structure of lithium were performed using the method of tight-binding. No approximations were made in computing the integrals. The results of this work, as will be shown, agree very well with those

obtained by the Green's Function method,[9] the Composite Waves method,[10] and a method of Modified Plane Waves.[11] Both the methods of Composite Waves and of Modified Plane Waves are variations of the method of Augmented Plane Waves.

CHAPTER II

THE CRYSTAL POTENTIAL

In band theory, each electron is considered to move in a periodic potential field. Similar to the Hartree-Fock approach to the free atom, this potential is assumed to be the average effect of all electron-electron and electron-nuclei interactions. Due to this averaging, the potential experienced by each electron is only a function of its position in the crystal and is not a function of the coordinates of the other electrons. Further, it is customary to assume that all electrons of the crystal experience the same potential. Such an assumption is only qualitatively correct but since no extensive self-consistent calculations of the crystalline potential have yet been performed, the potentials themselves are only approximately correct. At the present time, crystal potentials are obtained mainly by analogy to the free atom and by physical intuition.

The potential used in this calculation is a "flattened" or "muffin-tin" version of the Seitz potential.[12] The Seitz potential for the lithium crystal was constructed by Seitz from the spherical potential for an isolated lithium atom. Certain algebraic mistakes of Seitz were later corrected by Kohn and Rostocker.[13]

In the "muffin-tin" approximation, the Wigner-Seitz cell is divided into two regions by an inscribed sphere. Within the inscribed sphere the Seitz potential is used. Exterior to the inscribed sphere, but interior to the cell boundary, a potential of constant value $\bar{V}$ is used, this constant being chosen equal to the average value of the Seitz potential within this region. For ease of computation, the tabular form of the Seitz potential as published by Kohn and Rostocker [13] is replaced by a polynomial which has been fitted to the tabular function by the method of least squares. The resulting expression is

$$V(r) = \sum_{n=-1}^{n=+7} C_n r^n, \qquad (9)$$

where

$$C_{-1} = -2.9258671$$

$$C_0 = 2.7018157$$

$$C_1 = 1.6756787$$

$$C_2 = -6.823063$$

$$C_3 = 6.8323735$$

$$C_4 = -3.4872725$$

$$C_5 = 0.9885456$$

$$C_6 = -0.1479572$$

$$C_7 = 0.0091263 .$$

Table 1 gives a comparison between the tabular Seitz potential and its curve fit.

In calculating $\bar{V}$, the average value of the Seitz potential between the inscribed sphere and the cell boundary, the Seitz potential in this region was

Table 1

Curve Fit for the
Seitz Potential

r	-rV(r) Tabulated	Curve fit
0.02	2.8635	2.8712
0.04	2.7720	2.8155
0.06	2.7250	2.7591
0.08	2.6755	2.7022
0.10	2.6265	2.6451
0.12	2.5785	2.5880
0.14	2.5290	2.5310
0.16	2.4800	2.4745
0.18	2.4310	2.4185
0.20	2.3810	2.3632
0.24	2.2815	2.2509
0.28	2.1800	2.1513
0.32	2.0792	2.0523
0.36	1.9731	1.9587
0.40	1.8680	1.8707
0.44	1.7714	1.7886
0.48	1.6898	1.7124
0.52	1.6208	1.6416
0.56	1.5604	1.5777

r	11 $-rV(r)$ Tabulated	Curve Fit
0.60	1.5069	1.5189
0.68	1.4171	1.4172
0.76	1.3441	1.3347
0.84	1.2831	1.2689
0.92	1.2121	1.2171
1.00	1.1883	1.1766
1.08	1.1529	1.1450
1.16	1.1229	1.1203
1.24	1.1018	1.1006
1.32	1.0830	1.0847
1.40	1.0675	1.0713
1.48	1.0545	1.0598
1.64	1.0348	1.0409
1.80	1.0233	1.0262
1.96	1.0162	1.0159
2.12	1.0144	1.0101
2.28	1.0146	1.0020
2.44	1.0114	1.0088
2.60	1.0062	1.0094
2.76	1.0032	1.0081
2.92	1.0016	1.0043
3.08	1.0008	0.9993

r	$-rV(r)^{12}$ Tabulated	Curve Fit
3.24	1.0004	0.9963
3.40	1.0002	0.9986
3.56	1.0001	1.0044
3.72	1.0000	0.9987

fitted by the polynomial

$$V(r) = \frac{1}{\alpha_0} \left\{ \frac{\alpha_1}{r} + \alpha_2 + \alpha_3 r + \alpha_4 r^2 \right\}, \tag{10}$$

where

$$\alpha_0 = 4.9152$$

$$\alpha_1 = 8.00563776$$

$$\alpha_2 = -2.8428$$

$$\alpha_3 = 0.8748$$

$$\alpha_4 = -0.0900 .$$

Following Ham, the cell boundary is then approximated by that of the equivalent volume sphere giving

$$\bar{V} = \frac{\int_{R_{IS}}^{R_{EVS}} V(r)\, r^2 dr}{\int_{R_{IS}}^{R_{EVS}} r^2 dr} . \tag{11}$$

where R_{IS} and R_{EVS} are the radii of the inscribed and equivalent volume spheres respectively, viz.

$$R_{IS} = \frac{\sqrt{3}}{4} a_0$$

$$R_{EVS} = \frac{1}{2} \left(\frac{3}{\pi} \right)^{1/3} a_0 . \tag{12}$$

For $a_0 = 6.65$ au, this procedure yields

$$\bar{V} = -0.3248 \text{ au} . \tag{13}$$

To simplify calculations, the muffin-tin potential is now divided into two separate terms

$$V(\vec{r}) = V'(\vec{r}) + \bar{V} . \tag{14}$$

within the inscribed spheres, $V'(\vec{r})$ differs from the Seitz potential by a constant. Between the inscribed spheres $V'(\vec{r})$ is equal to zero. $V'(\vec{r})$ is now expanded in a Fourier series, viz.

$$V'(\vec{r}) = \sum_{\nu} V'_{\vec{K}_\nu} e^{i\vec{K}_\nu \cdot \vec{r}} = \sum_{\nu} V'_{\vec{K}_\nu} \cos \vec{K}_\nu \cdot \vec{r} \, . \tag{15}$$

Where the summation is taken over all sites in the reciprocal lattice and where use has been made of the relation,

$$V'(-\vec{r}) = V'(\vec{r}) \, . \tag{16}$$

The Fourier coefficients can be expressed as

$$V'_{\vec{K}_\nu} = \frac{1}{\Omega} \int_{\text{unit cell}} V'(\vec{r}) \cos \vec{K}_\nu \cdot \vec{r} \, d\tau \, . \tag{17}$$

Where

$$\Omega = a_0^3/2 \tag{18}$$

is the volume of the unit cell. Using the fact that $V'(\vec{r})$ is spherically symmetric within each inscribed sphere and zero in the region between the inscribed spheres, the expression for the Fourier ccefficients of $V'(\vec{r})$ becomes

$$V'_{K_\nu} = \frac{8\pi}{a_0^3 K_\nu} \int_{}^{R_{IS}} r V'(r) \sin K_\nu r \, dr \, . \tag{19}$$

Upon substitution of a polynomial expression for $V'(r)$, the above integral is easily performed. The resulting coefficients are tabulated in Table 2.

It should be emphasized at this point that the method of solution presented here is not restricted to such a "flattened" or "muffin tin" potential. This form of the potential was chosen only in order that comparison could be made with

Table 2

Fourier Coefficients for $V'(\vec{r})$

$\frac{a_0\vec{K}}{2\pi} = \vec{\ell}$			Fourier Coefficients
ℓ_x	ℓ_y	ℓ_z	V'_{K_ν}
0	0	0	-0.17391810
1	1	0	-0.08490524
2	0	0	-0.04674083
2	1	1	-0.03162225
2	2	0	-0.02576319
3	1	0	-0.02294729
2	2	2	-0.02078330
3	2	1	-0.01862729
4	0	0	-0.01650122
3	3	0	-0.01458237
4	1	1	-0.01458237
4	2	0	-0.01300156
3	3	2	-0.01179467
4	2	2	-0.01091941
4	3	1	-0.01029094
5	1	0	-0.01029094
5	2	1	-0.00940982
4	4	0	-0.00901830

$\frac{a_0\vec{K}}{2\pi} = \vec{\ell}$			Fourier Coefficients
ℓ_x	ℓ_y	ℓ_z	V'_{K_ν}
4	3	3	-0.008609158
5	3	0	-0.008609158
4	4	2	-0.008173826
6	0	0	-0.008173826
5	3	2	-0.007719871
6	1	1	-0.007719871
6	2	0	-0.007263887
5	4	1	-0.006825224
6	2	2	-0.006421279
6	3	1	-0.006064577
4	4	4	-0.005761505
5	5	0	-0.005512363
5	4	3	-0.005512363
7	1	0	-0.005512363
6	4	0	-0.005312334
6	3	3	-0.005152956
5	5	2	-0.005152956
7	2	1	-0.005152956
6	4	2	-0.005023771
7	3	0	-0.004913867

$\frac{a_0\vec{K}}{2\pi} = \vec{\ell}$			Fourier Coefficients
ℓ_x	ℓ_y	ℓ_z	V'_{K_y}
6	5	1	-0.004713354
7	3	2	-0.004713354
8	0	0	-0.004608399
5	5	4	-0.004494758
7	4	1	-0.004494758
8	1	1	-0.004494758
6	4	4	-0.004371255
8	2	0	-0.004371255
6	5	3	-0.004238740
6	6	0	-0.004099620
8	2	2	-0.004099620
7	4	3	-0.003957315
7	5	0	-0.003957315
8	3	1	-0.003957315
6	6	2	-0.003815717
7	5	2	-0.003678709
8	4	0	-0.003549757
8	3	3	-0.003431626
9	1	0	-0.003431626

the methods of modified plane waves, [11] composite waves, [10] and Green's function [9] which have been previously reported in the literature.

CHAPTER III

GROUP THEORY

Let η be an operator with a set of eigenfunctions $\Psi_{nr}(X_1, X_2, \ldots, X_s)$ such that

$$\eta \Psi_{nr}(\vec{X}) = \varepsilon_n \Psi_{nr}(\vec{X}). \tag{20}$$

The degeneracy associated with any eigenvalue ε_n is indicated by the subscript r. Thus for an m-fold degenerate eigenvalue ε_n, there are m linearly independent eigenfunctions $\Psi_{n1}, \Psi_{n2}, \ldots, \Psi_{nm}$. Due to the linear nature of Eq. (20), any linear combination of these m functions is also a solution corresponding to the eigenvalue ε_n and conversely, any acceptable solution ϕ of Eq. (20) corresponding to an m fold degenerate eigenvalue ε_n can be expressed as a linear combination of the m functions Ψ_{nr}, $r = 1, \ldots, m$.

To determine the effects of symmetry on the nature of the solutions $\Psi_{nr}(\vec{X})$, consider a group G of operations which leave the operator η and its eigenvalues ε_n invariant. Let the elements of G be denoted by $\mathcal{R}$ when they act on the coordinates $X_1, \ldots, X_s$ and by $O_{\mathcal{R}}$ when they act on functions of these coordinates. Then, for all $\mathcal{R}$ contained in G,

$$O_{\mathcal{R}} (\eta - \varepsilon_n) \Psi_{nr}(\vec{X}) = (\eta - \varepsilon_n) O_{\mathcal{R}} \Psi_{nr}(\vec{X}) = 0, \tag{21}$$

and hence the functions $O_{\mathcal{R}} \Psi_{nr}(\vec{X})$ are eigenfunctions corresponding to the eigenvalue ε_n. From this it follows that, for all $\mathcal{R}$ contained in G, each and every one of the functions $O_{\mathcal{R}} \Psi_{nr}(\vec{X})$ can be expressed as a linear combination of all the m functions $\Psi_{nr}(\vec{X})$, i.e.

$$O_{\mathcal{R}} \Psi_{nr}(\vec{X}) = \sum_{r'} \Psi_{nr'}(\vec{X}) D_{r'r}(\mathcal{R}). \tag{22}$$

For a group G of order g, there will be g matrices $D_{r'r}(\mathcal{R})$, i.e., one for each element $\mathcal{R}$ contained in G. Thus the m wave functions $\Psi_{nr}(\vec{X})$ for each m-fold degenerate eigenvalue ε_n form the basis of a representation of the group G. In general, such a representation is reducible but it is clear that as more and more of the symmetry operations of η are included in G, thereby increasing the order g, the representations $D_{r'r}(\mathcal{R})$ of G come closer and closer to being irreducible. Presumably, if all the symmetry operations of η were included in G, the m eigenfunctions $\Psi_{nr}(\vec{X})$ corresponding to the m-fold degenerate eigenvalue ε_n would form an irreducible representation of the group G. This group of all possible symmetry operations of η is called the full symmetry group and is designated here as G_s. The eigenvalues and eigenfunctions can be labeled by the irreducible representation to which they belong. In such a case, the eigenvalues are labeled as $\varepsilon_{n\ell}$ and the eigenfunctions as $\Psi_{n\ell m}(\vec{X})$ where the subscripts n and ℓ denote the nth occurrence of the ℓth irreducible representation and where the subscript m defines $\Psi_{n\ell m}(\vec{X})$ as transforming under the operations of G_s as the mth row of the ℓth irreducible representation. In many cases it is neither necessary nor desirable to include all the symmetry operations of η in G. In such a case, the group G is a

subgroup of G_s, and it becomes possible for more than one irreducible representation to correspond to the same eigenvalue i.e. $\epsilon_{n'\ell'} = \epsilon_{n\ell}$. In such a case, it is customary to still label the eigenfunctions and eigenvalues by the irreducible representations of G with the understanding that there may exist additional symmetry-based degeneracy among these irreducible representations. Thus, from symmetry considerations alone, a great deal of information is obtained concerning the eigenvalue structure and the transformation properties of acceptable eigenfunctions.

In the particular case of crystal energy band theory, each electron is assumed to move in a periodic crystalline potential field $V(\vec{r})$ due to the averaged effects of exchange and coulomb interactions with all the other electrons and nuclei in the crystal. Using such an averaged potential, a one-electron Schrodinger equation can be written for each electron viz.

$$\left[-\frac{1}{2}\nabla^2 + V(\vec{r}) - E_\nu\right] \Psi_\nu(\vec{r}) = 0. \qquad (23)$$

In order to determine the structuring of the energy levels and the transformation properties of the $\Psi_\nu(\vec{r})$, it is only necessary to investigate the symmetry properties of the operator

$$\eta = \left[-\frac{1}{2}\nabla^2 + V(\vec{r}) - E_\nu\right]. \qquad (24)$$

This operator has both translational and rotational symmetry. The group of all spatial symmetry operations is called the space group and a general element of the space group for lithium can be represented by $\{\alpha | \vec{R}_n\}$ where α represents some proper or improper rotation of the coordinate system, and $\vec{R}_n$ represents some primitive translation of the coordinate system by

$$\vec{R}_n = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3 \qquad (25)$$

The product of two successive operations $\{\alpha|\vec{R}_{\vec{n}}\}$ and $\{\beta|\vec{R}_{\vec{m}}\}$ is defined by

$$\{\alpha|\vec{R}_{\vec{n}}\}\ \{\beta|\vec{R}_{\vec{m}}\} = \{\alpha\beta|\alpha\ \vec{R}_{\vec{m}} + \vec{R}_{\vec{n}}\}. \tag{26}$$

The translation group composed of the elements $\{\varepsilon|\vec{R}_{\vec{n}}\}$ is a subgroup of the space group and determines the transformation properties of the $\Psi_\nu(\vec{r})$ under translation. That is to say, an acceptable eigenfunction $\Psi_\nu(\vec{r})$ must transform under pure translation as a member of some irreducible representation of the translation group. Using Eq. (26), the product of two members of the translation group is seen to yield

$$\{\varepsilon|\vec{R}_{\vec{n}}\}\ \{\varepsilon|\vec{R}_{\vec{m}}\} = \{\varepsilon|\vec{R}_{\vec{n}} + \vec{R}_{\vec{m}}\} = \{\varepsilon|\vec{R}_{\vec{m}}\}\{\varepsilon|\vec{R}_{\vec{n}}\}. \tag{27}$$

Thus the translation group is abelian and all irreducible representations are one-dimensional. If this abelian group is required to be finite, then there must exist an integer N, however large, such that

$$\{\varepsilon|\vec{a}_1\}^N = \{\varepsilon|\vec{a}_2\}^N = \{\varepsilon|\vec{a}_3\}^N = \{\varepsilon|\vec{0}\}. \tag{28}$$

Since any irreducible representation of $\{\varepsilon|\vec{0}\}$ is a 1x1 unit matrix, this yields

$$\begin{aligned}\{\varepsilon|\vec{a}_1\} &= e^{i\frac{2\pi}{N}p_1}\\ \{\varepsilon|\vec{a}_2\} &= e^{i\frac{2\pi}{N}p_2}\\ \{\varepsilon|\vec{a}_3\} &= e^{i\frac{2\pi}{N}p_3}\end{aligned} \tag{29}$$

where p_1, p_2, and p_3 can assume any integer value from 0 to N-1. From Eq. (29) it is seen that the irreducible representations of a general element $\{\varepsilon|\vec{R}_{\vec{n}}\}$ of the translation group is given by

$$\{\varepsilon|\vec{R}_{\vec{n}}\} = \{\varepsilon|\vec{a}_1\}^{n_1}\{\varepsilon|\vec{a}_2\}^{n_2}\{\varepsilon|\vec{a}_3\}^{n_3} = e^{i\frac{2\pi}{N}\{p_1n_1+p_2n_2+p_3n_3\}}. \tag{30}$$

The irreducible representations are labeled by the three integers p_1, p_2, p_3. These irreducible representations of the translation group can be written in a more

convenient and compact manner by defining

$$\vec{k} = k_1\vec{b}_1 + k_2\vec{b}_2 + k_3\vec{b}_3 \ , \tag{31}$$

where

$$k_i = \frac{p_i}{N} \ ,$$

and where the $\vec{b}_i$ are defined by

$$\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij} . \tag{32}$$

Using $\vec{k}$ defined in this way to label the irreducible representations of the translation group, these irreducible representations can be written as

$$\{\varepsilon | \vec{R}_n\} = e^{i\vec{k}\cdot\vec{R}_n} . \tag{33}$$

There is one irreducible representation for every value of k_1, k_2, and k_3 yielding a total of N^3 irreducible representations. In the limit as N goes to infinity, there is an irreducible representation corresponding to every vector in the region $0 \leq k_1 < 1$, $0 \leq k_2 < 1$, $0 \leq k_3 < 1$. This region in K space corresponds to a unit cell of a lattice of primitive translations

$$\vec{K}_m = m_1\vec{b}_1 + m_2\vec{b}_2 + m_3\vec{b}_3 . \tag{34}$$

This is just the reciprocal lattice of Chapter I and the corresponding Wigner-Seitz cell is designated as the Brillouin zone. Each point in the Brillouin zone labels an irreducible representation and every irreducible representation is represented in this collection of points. That points external to the Brillouin zone introduce no new representation can be seen from the fact that any point external to the Brillouin zone, say $\vec{k} = \vec{k}_0$ can be written as

$$\vec{k}_0 = \vec{k} + \vec{K}_m \tag{35}$$

where $\vec{K}_m$ is some reciprocal lattice vector and $\vec{k}$ is some point in the Brillouin zone. From Eqs. (32) and (34), it is seen that

$$e^{i\vec{k}_0 \cdot \vec{R}_n} = e^{i\vec{k} \cdot \vec{R}_n} . \qquad (36)$$

Thus the set of points $\vec{k} + \vec{K}_m$ all designate the same irreducible representation of the translation group and are said to be equivalent. By the same reasoning it is seen that no two points within the Brillouin zone can label the same irreducible representation since they cannot be connected by any primitive translation $\vec{K}_g$. The same, however, cannot be said for surface points since every point on the surface of the Brillouin zone is connected to at least one other surface point by a reciprocal lattice vector. This property is due to the fact that each surface point belongs to two or more Wigner-Seitz cells. Thus two or more surface points can designate the same irreducible representation and accordingly are called equivalent surface points. In order to eliminate this double valued nature the equivalent points are considered indistinguishable (different coordinates for the same point) or, alternatively, only one member of each set of equivalent surface points is considered to be contained in the Brillouin zone.

Since the irreducible representations of the translation group are known, the transformation properties of the $\Psi_\nu(\vec{r})$ under translation can now be determined. Let $O_{\vec{R}_n}$ be the function operator corresponding to the coordinate transformation $\{\varepsilon | \vec{R}_n\}$, then if $\Psi_\nu(\vec{r})$ transforms under translation as the basis of the irreducible representation designated by $\vec{k}$, then

$$O_{\vec{R}_n} \Psi_\nu(\vec{r}) = \Psi_\nu(\vec{r} + \vec{R}_n) = e^{i\vec{k} \cdot \vec{R}_n} \Psi_\nu(\vec{r}) \qquad . (37)$$

Thus one of the sets of indices contained in ν is $\vec{k}$ and an appropriate wave function is labeled as $\Psi_{\lambda,k}(\vec{r})$. Since the index $\vec{k}$ assumes a continuous range of

values it is customary to express $\Psi_{\lambda,\vec{k}}(\vec{r})$ as $\Psi_{\lambda}(\vec{k},\vec{r})$. The index $\vec{k}$ describes the transformation properties of the eigenfunction under translation and the set of indices λ designate different occurrences of the same irreducible representation of the translation group and also the transformation properties under rotation. The most general expression for $\Psi_{\lambda}(\vec{k},\vec{r})$ which satisfies the transformation requirements of Eq. (37) is

$$\Psi_{\lambda}(\vec{k},\vec{r}) = U_{\lambda}(\vec{k},\vec{r})\, e^{i\vec{k}\cdot\vec{r}}, \qquad (38)$$

where $U_{\lambda}(\vec{k},\vec{r})$ is periodic with the lattice

$$U_{\lambda}(\vec{k},\vec{r}+\vec{R}_n) = U_{\lambda}(\vec{k},\vec{r}). \qquad (39)$$

Such an expression is called the Bloch form of the wave function $\Psi_{\lambda}(\vec{k},\vec{r})$. Since $\vec{k}$ serves only to designate the irreducible representation of the translation group to which $\Psi_{\lambda}(\vec{k},\vec{r})$ belongs, and since $\vec{k}$ and $\vec{k}+\vec{K}_g$ label the same irreducible representation, it follows that

$$\Psi_{\lambda}(\vec{k}+\vec{K}_g,\vec{r}) = \Psi_{\lambda}(\vec{k},\vec{r}), \qquad (40)$$

and hence

$$U_{\lambda}(\vec{k}+\vec{K}_g,\vec{r}) = e^{-i\vec{K}_g\cdot\vec{r}}\, U_{\lambda}(\vec{k},\vec{r}). \qquad (41)$$

To determine the transformation properties of the $\Psi_{\lambda}(\vec{k},\vec{r})$ under rotations, it is convenient to use the Bloch form of the wave function and examine the transformation properties of the $U_{\lambda}(\vec{k},\vec{r})$. This has the effect of assuring that the wave functions possess the correct transformation properties under translation. If the Bloch form of Eq. (38) is substituted for $\Psi_{\nu}(\vec{r})$ into Eq. (23), the resulting differential equation is

$$\left[-\frac{1}{2}\nabla^2 + V(\vec{r}) - i\vec{k}\cdot\nabla + \frac{1}{2}k^2 - E_{\lambda}(\vec{k})\right] U_{\lambda}(\vec{k},\vec{r}) = 0. \qquad (42)$$

The transformation properties of the $U_\lambda(\vec{k}, \vec{r})$ are determined by the group G of spatial rotations $\mathcal{R}$, proper and improper, which leave the operator

$$\eta(\vec{k}, \vec{r}) = -\frac{1}{2}\nabla^2 + V(\vec{r}) - i\vec{k}\cdot\vec{\nabla} + \frac{1}{2}k^2 - E_\lambda(\vec{k}) \qquad (43)$$

invariant or which, for surface points of the Brillouin zone, transform $\eta(\vec{k}, \vec{r})$ into the equivalent operator $\eta(\vec{k} + \vec{K}_g, \vec{r})$ where $\vec{K}_g$ is a reciprocal lattice vector and where $|\vec{k}| = |\vec{k} + \vec{K}_g|$. This group G is a subgroup of the point group and is called the group of the wave vector--specifically, the group of the wave vector is composed of all operations $\{\alpha|\vec{0}\}$ which, when operating on the reciprocal coordinates, leaves the vector $\vec{k}$ invariant or which transforms $\vec{k}$ into $\vec{k} + \vec{K}_g$.

Thus, by symmetry arguments alone, it is found that an acceptable wave function must have the form

$$\psi_\nu(\vec{r}) = U_\lambda(\vec{k}, \vec{r})\, e^{i\vec{k}\cdot\vec{r}}, \qquad (44)$$

where the $U_\lambda(\vec{k}, \vec{r})$ must transform under rotation as the various members of the irreducible representations of the group of the wave vector.

CHAPTER IV

CONSTRUCTION OF THE WAVE FUNCTION

As mentioned previously, a crystalline wave function must possess certain transformation properties which are dictated by the translational and rotational symmetry of the crystal. Specifically, in order for a wave function to be considered acceptable, it must transform under translation as a member of an irreducible representation of the translation group and, under proper and improper spatial rotations, the periodic part of the wave function, as defined by Eq. (38), must transform as a member of an irreducible representation of the group of the wave vector. If such a wave function is to be represented by a linear combination of a set of basis functions, then these basis functions must be capable of combining together in such a manner as to possess the desired transformation properties under all the symmetry operations. The set of basis functions chosen for this work are the normalized Bloch functions

$$b_{n\ell m}(\vec{k}, \vec{r}) = [N \Omega_{n \ell m}(\vec{k})]^{-1/2} \sum_{\nu} e^{i\vec{k} \cdot \vec{R}_\nu} \phi_{n\ell m}(\vec{r} - \vec{R}_\nu), \quad (45)$$

where the summation is carried over all lattice sites of the crystal (schematically represented by N), and where the constant of normalization is given by $[N \Omega_{n \ell m}(\vec{k})]^{-1/2}$. As will be seen, the index $\vec{k}$ labels the irreducible

representation of the translation group to which $b_{n\ell m}(\vec{k}, \vec{r})$ belongs and the indices ℓ and m label the mth row of the ℓth irreducible representation of the three dimensional rotation group $\mathcal{O}(3)$ to which $b_{n\ell m}(\vec{k}, \vec{r})$ belongs if the $\phi_{n\ell m}(\vec{r})$ are properly chosen. Since the highest symmetry possible in the group of the wave vector is that of the point group of the crystal, all operations present in the group of the wave vector are also contained in $\mathcal{O}(3)$ and thus the periodic portion of a proper combination of the $b_{n\ell m}(\vec{k}, \vec{r})$ will transform like a member of some irreducible representation of the group of the wave vector.

To demonstrate that $b_{n\ell m}(\vec{k}, \vec{r})$ has the required transformation properties under translation, examine the function

$$b_{n\ell m}(\vec{k}, \vec{r} + \vec{R}_{\nu'}) = [N \Omega_{n\ell m}(\vec{k})]^{-1/2} \sum_{\nu} e^{i\vec{k} \cdot \vec{R}_{\nu}} \phi_{n\ell m}(\vec{r} + \vec{R}_{\nu'} - \vec{R}_{\nu}), \quad (46)$$

where $\vec{R}_{\nu'}$ is any primitive translation. Multiplying and dividing the right hand side of this expression by $e^{i\vec{k} \cdot \vec{R}_{\nu'}}$ yields

$$\begin{aligned} b_{n\ell m}(\vec{k}, \vec{r} + \vec{R}_{\nu'}) &= e^{i\vec{k} \cdot \vec{R}_{\nu'}} [N \Omega_{n\ell m}(\vec{k})]^{-1/2} \sum_{\nu} e^{i\vec{k} \cdot (\vec{R}_{\nu} - \vec{R}_{\nu'})} \phi_{n\ell m}[\vec{r} - (\vec{R}_{\nu} - \vec{R}_{\nu'})] \\ &= e^{i\vec{k} \cdot \vec{R}_{\nu'}} b_{n\ell m}(\vec{k}, \vec{r}). \end{aligned} \quad (47)$$

Thus the $b_{n\ell m}(\vec{k}, \vec{r})$ possess the correct transformation properties under translation.

To examine the transformation properties of $b_{n\ell m}(\vec{k}, \vec{r})$ under the coordinate operations $\mathcal{R}$ of the group of the wave vector, let $O_{\mathcal{R}}$ represent the corresponding function operator defined in the usual manner,[14] i.e.

$$O_{\mathcal{R}} f(\vec{r}) = f(\mathcal{R}^{-1} \vec{r}).$$

Then

$$O_{\mathcal{R}} b_{n\ell m}(\vec{k}, \vec{r}) = [N \Omega_{n\ell m}(\vec{k})]^{-1/2} \sum_{\nu} e^{i\vec{k} \cdot \vec{R}_{\nu}} \phi_{n\ell m}(\mathcal{R}^{-1} \vec{r} - \vec{R}_{\nu}). \quad (48)$$

Since the group of the wave vector is a subgroup of the point group of the crystal,

all operations $\mathcal{R}$ of the group of the wave vector leave the crystal invariant and hence when $\mathcal{R}$ operates on a translation vector $\vec{R}_\nu$, the result is another translation vector $\vec{R}_{\nu'}$, viz.

$$\mathcal{R}\,\vec{R}_\nu = \vec{R}_{\nu'}.$$

Thus

$$O_{\mathcal{R}} b_{n\ell m}(\vec{k}, \vec{r}) = [N\Omega_{n\ell m}(\vec{k})]^{-1/2} \sum_{\nu'} e^{i\vec{k}\cdot\mathcal{R}^{-1}\vec{R}_{\nu'}} \phi_{n\ell m}\{\mathcal{R}^{-1}(\vec{r} - \vec{R}_{\nu'})\}. \quad (49)$$

Since $\mathcal{R}$ is a member of the group of the wave vector

$$e^{i\vec{k}\cdot\mathcal{R}^{-1}\vec{R}_{\nu'}} = e^{i\mathcal{R}\vec{k}\cdot\mathcal{R}\mathcal{R}^{-1}\vec{R}_{\nu'}} = e^{i\mathcal{R}\vec{k}\cdot\vec{R}_{\nu'}} = e^{i\vec{k}\cdot\vec{R}_{\nu'}}. \quad (50)$$

Upon substituting this into Eq. (49), this yields

$$O_{\mathcal{R}} b_{n\ell m}(\vec{k}, \vec{r}) = [N\Omega_{n\ell m}(\vec{k})]^{-1/2} \sum_{\nu'} e^{i\vec{k}\cdot\vec{R}_{\nu'}} \phi_{n\ell m}\{\mathcal{R}^{-1}(\vec{r} - \vec{R}_{\nu'})\}. \quad (51)$$

Hence the $b_{n\ell m}(\vec{k}, \vec{r})$ possess the same transformation properties as the $\phi_{n\ell m}(\vec{r})$ under the operations of the group of the wave vector. Thus if the $\phi_{n\ell m}(\vec{r})$ are constructed so as to transform as members of the irreducible representations of $\mathcal{O}(3)$, then the $b_{n\ell m}(\vec{k}, \vec{r})$ will possess like transformation properties.

In order for the $b_{n\ell m}(\vec{k}, \vec{r})$ to form an acceptable set of basis functions for any and all points in the Brillouin zone, it must be possible for each and every value of $\vec{k}$ to combine the given set of Bloch sums in such a manner that the periodic portion of this combination transforms as the desired member of some irreducible representation of the group of the wave vector. Since any given group of the wave vector is a subgroup of $\mathcal{O}(3)$, this requirement will be met if sufficient values of ℓ are represented in the Bloch set and if all the $2\ell+1$ values of m are included for each choice of ℓ.

The spherical harmonics $Y_\ell^m(\theta, \phi)$ form a basis for the irreducible

representations of $\mathcal{O}(3)$ and hence the $b_{n\ell m}(\vec{k},\vec{r})$ can be written as

$$b_{n\ell m}(\vec{k},\vec{r}) = [N\Omega_{n\ell m}(\vec{k})]^{-1/2} \sum_{\nu} e^{i\vec{k}\cdot\vec{R}_\nu} \phi_{n\ell}(|\vec{r}-\vec{R}_\nu|) Y_\ell^m(\theta_\nu,\phi_\nu). \tag{52}$$

The selection of the $\phi_{n\ell}(r)$ is not dictated by symmetry and is left entirely up to the discretion of the investigator. It is desirable that these $\phi_{n\ell}(r)$ be so chosen that only a small number of basis functions are required to yield a good approximation of the wave function for any given point in the Brillouin zone. In choosing such a set of $\phi_{n\ell}(r)$ it is instructive to investigate the case of an expanded crystal where the internuclear separation is much greater than the effective radius of the free atom. In this case there is little overlap between the orbitals of neighboring atoms and the wave functions of the different bands of the crystal are given to an excellent degree of approximation by

$$\begin{aligned}
\Psi_{1A}(\vec{k},\vec{r}) &= b_{100}(\vec{k},\vec{r}),\\
\Psi_{2A}(\vec{k},\vec{r}) &= b_{200}(\vec{k},\vec{r}),\\
\Psi_{2\lambda}(\vec{k},\vec{r}) &= \alpha_1 b_{21-1}(\vec{k},\vec{r}) + \beta_1 b_{210}(\vec{k},\vec{r}) + \gamma_1 b_{211}(\vec{k},\vec{r}),\\
\Psi_{2\sigma}(\vec{k},\vec{r}) &= \alpha_2 b_{21-1}(\vec{k},\vec{r}) + \beta_2 b_{210}(\vec{k},\vec{r}) + \gamma_2 b_{211}(\vec{k},\vec{r}),\\
\Psi_{2\delta}(\vec{k},\vec{r}) &= \alpha_3 b_{21-1}(\vec{k},\vec{r}) + \beta_3 b_{210}(\vec{k},\vec{r}) + \gamma_3 b_{211}(\vec{k},\vec{r}),
\end{aligned} \tag{53}$$

etc., where the subscript A denotes the one dimensional identity representation of the group of the wave vector, the subscripts λ, σ, δ denote a member of some particular irreducible representation of the group of the wave vector and where the coefficients α_i, β_i, γ_i are entirely determined by the symmetry of the problem and by the requirement of normalization. For this type of expanded crystal, the most appropriate choice for the $\phi_{n\ell}(r)$ is that of the Hartree-Fock radial functions

for the free atom. For obvious reasons, such a situation as that described above is called the case of tight-binding. For smaller values of internuclear separation the overlap between orbitals of neighboring atoms is no longer negligible and the wave functions given above become only approximate. To the first order, the perturbation due to the interaction between neighboring atoms can be said to cause a mixing between those wave functions of the same $\vec{k}$ belonging to different occurrences of the same members of the same irreducible representation of the group of the wave vector. As to whether or not this perturbation can be treated as simply effecting a mixing of adjacent states of the same symmetry depends on the detail nature and magnitude of this interaction.

The method of Linear Combination of Atomic Orbitals (LCAO) in molecular physics is a direct adaption of the procedure of tight-binding. The success of LCAO in molecular work leads one to expect similar success using the method of tight-binding in solid state problems.

In the case of the conduction band of lithium, the bases chosen are the five normalized Bloch sums

$$
\begin{aligned}
b_{1s}(\vec{k},\vec{r}) &= [N\Omega_{1s}(\vec{k})]^{-1/2} \sum_{\nu} e^{i\vec{k}\cdot\vec{R}_\nu}\ \phi_{1s}(\vec{r}-\vec{R}_\nu) \\
b_{2s}(\vec{k},\vec{r}) &= [N\Omega_{2s}(\vec{k})]^{-1/2} \sum_{\nu} e^{i\vec{k}\cdot\vec{R}_\nu}\ \phi_{2s}(\vec{r}-\vec{R}_\nu) \\
b_{2p_x}(\vec{k},\vec{r}) &= [N\Omega_{2p_x}(\vec{k})]^{-1/2} \sum_{\nu} e^{i\vec{k}\cdot\vec{R}_\nu}\ \phi_{2p_x}(\vec{r}-\vec{R}_\nu) \\
b_{2p_y}(\vec{k},\vec{r}) &= [N\Omega_{2p_y}(\vec{k})]^{-1/2} \sum_{\nu} e^{i\vec{k}\cdot\vec{R}_\nu}\ \phi_{2p_y}(\vec{r}-\vec{R}_\nu) \\
b_{2p_z}(\vec{k},\vec{r}) &= [N\Omega_{2p_z}(\vec{k})]^{-1/2} \sum_{\nu} e^{i\vec{k}\cdot\vec{R}_\nu}\ \phi_{2p_z}(\vec{r}-\vec{R}_\nu)
\end{aligned}
\qquad (54)
$$

where the radial parts of the ϕ functions are taken to be the Hartree-Fock solutions for the free atom and where the angular parts of the functions ϕ_{2p_x}, ϕ_{2p_y},

ϕ_{2p_z} are constructed from the spherical harmonics Y_1^{-1}, Y_1^{0}, Y_1^{+1} in the usual manner.

The Hartree-Fock functions for the 1s, 2s, and 2p states of lithium have been published in tabular form by V. Fock and M. Petrashen.[15] Analytic expressions for these tabular functions can be obtained by the method of least squares.[16] The resulting functions are

$$\begin{aligned}
\phi_{1s}(\vec{r}) &= \alpha_{11s} e^{-\alpha 21s r} + \alpha_{31s} e^{-\alpha 41s r}, \\
\phi_{2s}(\vec{r}) &= \alpha_{12s} e^{-\alpha 22s r} + \alpha_{32s} r e^{-\alpha 42s r}, \\
\phi_{2p_x}(\vec{r}) &= x\,[\alpha_{12p} e^{-\alpha 22p r} + \alpha_{32p} e^{-\alpha 42p r}], \\
\phi_{2p_y}(\vec{r}) &= y\,[\alpha_{12p} e^{-\alpha 22p r} + \alpha_{32p} e^{-\alpha 42p r}], \\
\phi_{2p_z}(\vec{r}) &= z\,[\alpha_{12p} e^{-\alpha 22p r} + \alpha_{32p} e^{-\alpha 42p r}],
\end{aligned} \tag{55}$$

where

$\alpha_{11s} = 1.91049$	$\alpha_{12s} = 0.367485$	$\alpha_{12p} = 0.107199$
$\alpha_{21s} = 2.4423$	$\alpha_{22s} = 2.222$	$\alpha_{22p} = 0.5166$
$\alpha_{31s} = 0.701005$	$\alpha_{32s} = -0.120003$	$\alpha_{32p} = 0.0757334$
$\alpha_{41s} = 4.5531$	$\alpha_{42s} = 0.6632$	$\alpha_{42p} = 1.9662$

A comparison of the curve fits with the actual tabular functions is given in Tables 3 and 4.

Table 3

Comparison of Tabular and Curve Fit Functions for $\sqrt{4\pi}\, r\phi_{1S}(\vec{r})$

r	Tabular	Curve fit
0.00	0.0000	0.0000
0.02	0.1744	0.1744
0.04	0.3286	0.3285
0.06	0.4645	0.4644
0.08	0.5838	0.5837
0.10	0.6882	0.6881
0.12	0.7790	0.7789
0.14	0.8576	0.8575
0.16	0.9251	0.9250
0.18	0.9825	0.9825
0.20	1.0310	1.0310
0.22	1.0714	1.0714
0.24	1.1044	1.1044
0.26	1.1308	1.1309
0.28	1.1513	1.1514
0.30	1.1665	1.1667
0.32	1.1770	1.1771
0.34	1.1832	1.1833
0.36	1.1856	1.1857

r	Tabular	Curve fit
0.38	1.1846	1.1847
0.40	1.1806	1.1807
0.45	1.1595	1.1595
0.50	1.1262	1.1261
0.55	1.0840	1.0838
0.60	1.0358	1.0356
0.65	0.9839	0.9836
0.70	0.9298	0.9295
0.75	0.8748	0.8746
0.80	0.8200	0.8199
0.85	0.7661	0.7661
0.90	0.7137	0.7138
0.95	0.6633	0.6633
1.00	0.6149	0.6151
1.10	0.5254	0.5257
1.20	0.4460	0.4462
1.30	0.3764	0.3766
1.40	0.3161	0.3163
1.50	0.2644	0.2645
1.60	0.2203	0.2204
1.70	0.1830	0.1829
1.80	0.1515	0.1515

r	Tabular	Curve fit
1.90	0.1251	0.1250
2.00	0.1031	0.1030
2.20	0.0696	0.0694
2.40	0.0467	0.0464
2.60	0.0311	0.0308
2.80	0.0206	0.0203
3.00	0.0136	0.0134
3.20	0.0090	0.0087
3.40	0.0059	0.0057
3.60	0.0039	0.0037
3.80	0.0026	0.0024
4.00	0.0017	0.0015
4.40	0.0007	0.0006
4.80	0.0001	0.0003

Table 4

Comparison of Tabular and Curve Fit Functions for $\sqrt{4\pi}\, r\, \phi_{2S}(\vec{r})$ and for $\sqrt{4\pi/3}\, \frac{r^2}{x}\, \phi_{2p_x}(\vec{r})$

	$\sqrt{4\pi}\, r\, \phi_{2s}(\vec{r})$		$\sqrt{4\pi/3}\, \frac{r^2}{x}\, \phi_{2p_x}(\vec{r})$	
r	Tabular	Curve Fit	Tabular	Curve Fit
0.00	0.0000	0.0000	0.0000	0.0000
0.02	0.0271	0.0248	0.0001	0.0001
0.04	0.0510	0.0470	0.0006	0.0006
0.06	0.0720	0.0669	0.0014	0.0013
0.08	0.0904	0.0847	0.0024	0.0022
0.10	0.1064	0.1003	0.0036	0.0034
0.12	0.1201	0.1141	0.0051	0.0047
0.14	0.1317	0.1260	0.0068	0.0063
0.16	0.1415	0.1363	0.0087	0.0081
0.18	0.1497	0.1450	0.0107	0.0100
0.20	0.1562	0.1522	0.0129	0.0121
0.22	0.1612	0.1580	0.0152	0.0144
0.24	0.1648	0.1625	0.0176	0.0167
0.26	0.1673	0.1659	0.0202	0.0193
0.28	0.1688	0.1681	0.0229	0.0219
0.30	0.1692	0.1693	0.0257	0.0247
0.32	0.1685	0.1695	0.0285	0.0275
0.34	0.1671	0.1688	0.0315	0.0305

r	$\sqrt{4\pi}\, r\, \phi_{2s}(\vec{r})$ Tabular	$\sqrt{4\pi}\, r\, \phi_{2s}(\vec{r})$ Curve Fit	$\sqrt{4\pi/3}\, \frac{r^2}{x}\, \phi_{2p_x}(\vec{r})$ Tabular	$\sqrt{4\pi/3}\, \frac{r^2}{x}\, \phi_{2p_x}(\vec{r})$ Curve Fit
0.36	0.1649	0.1673	0.0345	0.0335
0.38	0.1620	0.1650	0.0376	0.0367
0.40	0.1584	0.1620	0.0408	0.0399
0.45	0.1471	0.1518	0.0490	0.0482
0.50	0.1328	0.1381	0.0575	0.0569
0.55	0.1162	0.1217	0.0663	0.0659
0.60	0.0978	0.1032	0.0753	0.0751
0.65	0.0780	0.0830	0.0845	0.0845
0.70	0.0571	0.0615	0.0939	0.0941
0.75	0.0355	0.0390	0.1033	0.1038
0.80	0.0134	0.0160	0.1129	0.1135
0.85	-0.0090	-0.0074	0.1225	0.1233
0.90	-0.0315	-0.0310	0.1322	0.1331
0.95	-0.0541	-0.0546	0.1419	0.1429
1.00	-0.0765	-0.0780	0.1516	0.1526
1.10	-0.1206	-0.1238	0.1710	0.1720
1.20	-0.1632	-0.1678	0.1901	0.1911
1.30	-0.2039	-0.2093	0.2090	0.2098
1.40	-0.2423	-0.2482	0.2275	0.2281
1.50	-0.2782	-0.2842	0.2454	0.2458
1.60	-0.3115	-0.3173	0.2628	0.2629

r	$\sqrt{4\pi}\, r\, \phi_{2s}(\vec{r})$ Tabular	Curve Fit	$\sqrt{4\pi/3}\, \frac{r^2}{x}\, \phi_{2p_x}(\vec{r})$ Tabular	Curve Fit
1.70	-0.3422	-0.3475	0.2796	0.2794
1.80	-0.3704	-0.3748	0.2957	0.2952
1.90	-0.3959	-0.3993	0.3110	0.3103
2.00	-0.4186	-0.4211	0.3255	0.3246
2.20	-0.4566	-0.4570	0.3521	0.3508
2.40	-0.4852	-0.4837	0.3752	0.3739
2.60	-0.5052	-0.5022	0.3949	0.3936
2.80	-0.5176	-0.5135	0.4112	0.4100
3.00	-0.5233	-0.5186	0.4241	0.4232
3.20	-0.5232	-0.5183	0.4338	0.4332
3.40	-0.5183	-0.5135	0.4406	0.4403
3.60	-0.5093	-0.5084	0.4446	0.4446
3.80	-0.4970	-0.4931	0.4460	0.4463
4.00	-0.4819	-0.4788	0.4450	0.4457
4.40	-0.4462	-0.4447	0.4371	0.4382
4.80	-0.4060	-0.4061	0.4226	0.4239
5.20	-0.3642	-0.3656	0.4031	0.4045
5.60	-0.3229	-0.3252	0.3802	0.3815
6.00	-0.2835	-0.2864	0.3551	0.3561
6.40	-0.2468	-0.2499	0.3288	0.3295
6.80	-0.2132	-0.2164	0.3022	0.3025

r	$\sqrt{4\pi}\, r\, \phi_{2s}(\vec{r})$ Tabular	Curve Fit	$\sqrt{4\pi/3}\, \frac{r^2}{x}\, \phi_{2p_x}(\vec{r})$ Tabular	Curve Fit
7.20	-0.1830	-0.1860	0.2758	0.2759
7.60	-0.1562	-0.1590	0.2502	0.2500
8.00	-0.1326	-0.1351	0.2258	0.2253
9.00	-0.0830	-0.0881	0.1712	0.1701
10.00	-0.0551	-0.0560	0.1267	0.1253
11.00	-0.0346	-0.0349	0.0920	0.0904
12.00	-0.0213	-0.0214	0.0657	0.0642
13.00	-0.0136	-0.0130	0.0463	0.0449
14.00	-0.0079	-0.0077	0.0323	0.0311
15.00	-0.0051	-0.0046	0.0223	0.0213
16.00	-0.0028	-0.0027	0.0152	0.0145
17.00	-0.0018	-0.0016	0.0104	0.0097
18.00	-0.0010	-0.0009	0.0070	0.0065
19.00	-0.0006	-0.0005	0.0048	0.0043
20.00	-0.0003	-0.0003	0.0032	0.0022
21.00	-0.0002	-0.0002	0.0022	0.0019
22.00	-0.0001	-0.0001	0.0016	0.0012

CHAPTER V

THE SECULAR EQUATION

Using the set of Bloch tight-binding functions $b_{1s}(\vec{k},\vec{r})$, $b_{2s}(\vec{k},\vec{r})$, $b_{2p_x}(\vec{k},\vec{r})$, $b_{2p_y}(\vec{k},\vec{r})$, $b_{2p_z}(\vec{k},\vec{r})$ described in chapter IV, the conduction band wave function for any point in the Brillouin zone can be approximated by

$$\Psi_\lambda(\vec{k},\vec{r}) = a_\lambda^{1s}(\vec{k})b_{1s}(\vec{k},\vec{r}) + a_\lambda^{2s}(\vec{k})b_{2s}(\vec{k},\vec{r}) + a_\lambda^{2p_x}(\vec{k})b_{2p_x}(\vec{k},\vec{r}) + a_\lambda^{2p_y}(\vec{k})b_{2p_y}(\vec{k},\vec{r}) + a_\lambda^{2p_z}(\vec{k})b_{2p_z}(\vec{k},\vec{r}) \quad (56)$$

where $\vec{k}$ designates a particular irreducible representation of the translation group and where λ designates the transformation properties of the wave function under the operations of the group of the wave vector. Using the one electron Hamiltonian, H, Schrodinger's equation can be written as

$$[H - E_\lambda(\vec{k})]\,\Psi_\lambda(\vec{k},\vec{r}) = 0. \quad (57)$$

Multiplying this expression on the left by $b_\alpha^*(\vec{k},\vec{r})$ and integrating over $\vec{r}$ yields the five equations

$$\sum_\beta a_\lambda^\beta(\vec{k})\,[H_{\alpha,\beta}(\vec{k}) - E_\lambda(\vec{k})\,S_{\alpha,\beta}(\vec{k})] = 0 \quad (58)$$

where α and β take on the values 1s, 2s, $2p_x$, $2p_y$, $2p_z$, and where

$$H_{\alpha,\beta}(\vec{k}) = \int b_\alpha^*(\vec{k},\vec{r})\,H\,b_\beta(\vec{k},\vec{r})\,d\tau$$

$$S_{\alpha,\beta}(\vec{k}) = \int b_\alpha^*(\vec{k},\vec{r})\, b_\beta(\vec{k},\vec{r})\, d\tau. \qquad (59)$$

In order for these five equations to have a solution, they must possess a redundancy. This redundancy among the five equations leads to the secular equation

$$\det | H_{\alpha,\beta}(\vec{k}) - E_\lambda(\vec{k})\, S_{\alpha,\beta}(\vec{k})| = 0 \qquad (60)$$

For each value of $\vec{k}$, the solution of this equation will yield five allowed values for the energy $E_{\lambda i}(\vec{k})$ where the roots are arranged in order of ascending magnitude

$$E_{\lambda 1}(\vec{k}) \leq E_{\lambda 2}(\vec{k}) \leq E_{\lambda 3}(\vec{k}) \leq E_{\lambda 4}(\vec{k}) \leq E_{\lambda 5}(\vec{k}). \qquad (61)$$

For high symmetry values of $\vec{k}$, some of the $E_{\lambda I}(\vec{k})$ will be degenerate. If the 1s core electrons are assumed to experience the same potential field as the electrons of the conduction band, the lowest root, $E_{\lambda 1}(\vec{k})$, of the set $E_{\lambda i}(\vec{k})$ will correspond to the tightly bound 1s "band" and the corresponding wave function will be primarily $b_{1s}(\vec{k},\vec{r})$. The next higher root, $E_{\lambda 2}(\vec{k})$, will correspond to the conduction band and the corresponding wave function is assumed to be primarily of $b_{2s}(\vec{k},\vec{r})$, $b_{2p}(\vec{k},\vec{r})$, and $b_{1s}(\vec{k},\vec{r})$ character. The remaining roots correspond to higher energy bands of the crystal. Due to the small number of basis functions used in this calculation, these higher roots can be expected to yield only qualitative results at best.

In order to determine the roots of the secular equation, one must first determine the matrix elements $H_{\alpha,\beta}(\vec{k})$ and $S_{\alpha,\beta}(\vec{k})$. Using the relation

$$b_\gamma(\vec{k},\vec{r}) = [N\Omega_\gamma(\vec{k})]^{-1/2} \sum_\nu e^{i\vec{k}\cdot\vec{R}_\nu}\, \phi_\gamma(\vec{r}-\vec{R}_\nu), \qquad (62)$$

$H_{\alpha,\beta}(\vec{k})$ can be written as

$$H_{\alpha,\beta}(\vec{k}) = \frac{[\Omega_\alpha(\vec{k})\,\Omega_\beta(\vec{k})]^{-1/2}}{N} \sum_{\nu'}\sum_{\nu} e^{i\vec{k}\cdot(\vec{R}_\nu - \vec{R}_{\nu'})} \int \phi_\alpha^*(\vec{r}-\vec{R}_{\nu'}) H \phi_\beta(\vec{r}-\vec{R}_\nu)\, d\tau .$$

For each value of ν', the summation over ν yields the same result. Since the number of lattice sites in the crystal is represented schematically by N, the matrix element reduces to

$$H_{\alpha\beta}(\vec{k}) = [\Omega_\alpha(\vec{k})\Omega_\beta(\vec{k})]^{-1/2}\sum_\nu e^{i\vec{k}\cdot\vec{R}_\nu}\int\phi_\alpha^*(\vec{r})H\,\phi_\beta(\vec{r}-\vec{R}_\nu)\,d\tau$$
$$= [\Omega_\alpha(\vec{k})\Omega_\beta(\vec{k})]^{-1/2}\sum_\nu e^{i\vec{k}\cdot\vec{R}_\nu}\langle\phi_\alpha(\vec{0})\,|H|\,\phi_\beta(\vec{R}_\nu)\rangle. \qquad (63)$$

A similar reduction for $S_{\alpha\beta}(\vec{k})$ yields

$$S_{\alpha\beta} = [\Omega_\alpha(\vec{k})\Omega_\beta(\vec{k})]^{-1/2}\sum_\nu e^{i\vec{k}\cdot\vec{R}_\nu}\int\phi_\alpha(\vec{r})\,\phi_\beta(\vec{r}-\vec{R}_\nu)\,d\tau \qquad (64)$$
$$= [\Omega_\alpha(\vec{k})\Omega_\beta(\vec{k})]^{-1/2}\sum_\nu e^{i\vec{k}\cdot\vec{R}_\nu}\langle\phi_\alpha(\vec{0})|\,\phi_\beta(\vec{R}_\nu)\rangle.$$

Thus each matrix element is reduced to a sum over the crystal lattice of multi-center integrals. The term multi-center arises from the fact that the integrand consists of the product of an orbital centered about the origin, a function centered about the lattice site $\vec{R}_\nu$ and, perhaps, some third function centered about a third lattice site $\vec{R}_{\nu'}$. Using the expression

$$H = -\frac{1}{2}\nabla^2 + V'(\vec{r}) + \bar{V}, \qquad (65)$$

the basic multi-center integrals become

$$\langle\phi_\alpha(\vec{0})\,|\,\phi_\beta(\vec{R}_\nu)\rangle = \int\phi_\beta(\vec{r})\,\phi_\beta(\vec{r}-\vec{R}_\nu)\,d\tau,$$
$$\langle\phi_\alpha(\vec{0})\,|\,-\frac{1}{2}\nabla^2\,|\,\phi_\beta(\vec{R}_\nu)\rangle = \int\phi_\alpha(\vec{r})(-\frac{1}{2}\nabla^2)\phi_\beta(\vec{r}-\vec{R}_\nu)\,d\tau,$$
$$\langle\phi_\alpha(\vec{0})\,|\,V'\,|\,\phi_\beta(\vec{R}_\nu)\rangle = \int\phi_\alpha(\vec{r})\,V'(\vec{r})\,\phi_\beta(\vec{r}-\vec{R}_\nu)\,d\tau. \qquad (66)$$

These are called the integrals of overlap, kinetic energy, and potential energy respectively and are discussed in detail in later chapters.

An important feature of this reduction of matrix elements is that these basic two-center integrals are independent of the choice of $\vec{k}$ and hence need to

be calculated only once for each crystal. After all the necessary multi-center integrals have been calculated, the matrix elements of the secular equation associated with any given point in the Brillouin zone can be determined by merely performing the appropriate sums over the crystal lattice. Thus the energies and wave functions associated with any given point in the Brillouin zone can be quickly and easily determined. The method used in calculating these multi-center integrals is discussed in detail in chapter VI.

It is instructive to investigate the convergence of the summation over the crystal lattice site ν in Eqs. (63) and (64) for this is the point at which the customary nearest-neighbor approximation is introduced. For the matrix element $V'_{2p_x, 2s'}$ with $\vec{k} = \frac{2\pi}{a_0}$ (0.85,0,0), the summation over ν has been truncated at various distances from the origin corresponding to the inclusion of more and more sites. Values of this truncated sum are shown in Table 5. As can be seen, the summation does not begin to approach convergence until all sets of equivalent atoms up to the 25th nearest neighbor have been included. Table 5 also shows that there is a certain loss of significant figures in going from the basic integrals to the matrix elements. This difficulty was first pointed out by Parmenter,[17] but in this case the cancellation is not serious and appears to become significant only for the higher energy bands.

Table 5

Values of truncated summation of $V'_{2p_x,2s}$ for $\vec{k} = (2\pi/a_0)(0.85,0,0)$, $a_0 = 6.65$ au

Last Set of Nearest Neighbors included in Sum	Number of Equivalent Atoms in Set	Distance from Origin	Truncated sum[a] $V'_{2p_x,2s}$
0	1	0.000	0.0000
1	8	5.759	0.8632
2	6	6.650	0.1681
3	12	9.404	-1.3572
4	24	11.028	0.8624
5	8	11.518	0.0581
6	6	13.300	-0.1877
7	24	14.493	0.8531
8	24	14.870	0.0935
9	24	16.289	-0.4678
10	24	17.277	-0.2325
11	8	17.277	-0.0746
12	12	18.809	-0.1799
13	48	19.671	0.8531
14	24	19.950	-0.0706
15	6	19.950	-0.0784
16	24	21.029	-0.1149
17	24	21.803	-0.0442

Last Set of Nearest Neighbors included in Sum	Number of Equivalent Atoms in Set	Distance from Origin	Truncated sum[a] $V'_{2p_x,2s}$
18	24	22.055	-0.0781
19	8	23.036	-0.0944
20	24	23.745	-0.0711
21	24	23.745	-0.0717
22	24	23.977	-0.0875
23	48	24.882	-0.1144
24	24	25.540	-0.1006
25	48	25.540	-0.0944
26	6	26.600	-0.0933
27	24	27.216	-0.0903
28	24	27.419	-0.0957
29	24	27.419	-0.0939
30	12	28.213	-0.0947
31	24	28.213	-0.0941

[a]Since $V'_{2p_x,2s}$ is a pure imaginary number, the values listed are $V'_{2p_x,2s}/i$.

CHAPTER VI

CALCULATION OF MULTICENTER INTEGRALS

As shown in the previous chapter, the tight-binding matrix elements can be expressed in terms of a number of multicenter integrals of overlap, kinetic energy and potential energy. The overlap and kinetic energy integrals are a common occurrence in molecular work and many highly efficient methods have been developed to handle these integrals.[18-20] The same, however, cannot be said for the multicenter integrals of potential energy. Indeed, it is the intractability of these potential integrals which has heretofore imposed such drastic approximations in applying the method of tight-binding. The usual technique used in evaluating these potential integrals is to express the potential within each cell as $\mathcal{U}(\vec{r} - \vec{R}_\nu)$. Each term, $\mathcal{U}(\vec{r} - \vec{R}_\nu)$, reproduces the potential within the unit cell $\vec{R}_\nu$ and is zero elsewhere. The total potential can then be written as

$$V(\vec{r}) = \sum_{R_\nu} \mathcal{U}(\vec{r} - \vec{R}_\nu) \tag{67}$$

and each potential integral becomes a sum over the crystal lattice of three-center integrals. The most common approximation mentioned above is to assume that all potential integrals in which the two orbitals are separated by more than a fundamental lattice vector, $\vec{a}_i$, are negligible and to further assume in calculating these

integrals that the only three-center integrals which need to be considered are those in which the third center coincides with one of the orbital sites or lies in an adjacent cell. This is called the nearest neighbor approximation. For most crystals, this approximation is so drastic that the results, at best, are only qualitative.[6] In order to avoid such approximations in the present work, a new method of performing these potential integrals was devised. This new method is based on the technique of gaussian transformation[19] and proved to be so efficient that none of the above mentioned approximations was necessary. The formulation of these potential energy, overlap, and kinetic energy integrals is presented below.

A. Potential Energy Integrals.

In order to obtain expressions for the potential integrals

$$\langle \psi_\alpha^s(\vec{A}) \mid V' \mid \phi_\beta^s(\vec{B}) \rangle = \int \psi_\alpha^s(\vec{r}_A)\, V'(\vec{r})\, \phi_\beta^s(\vec{r}_B)\, d\tau , \tag{68}$$

involving two unnormalized Slater-type orbitals ψ_α^s and ϕ_β^s centered at lattice sites $\vec{A}$, and $\vec{B}$ respectively, it is convenient to employ a Fourier series expansion for $V'(\vec{r})$ as given in Eq. (15), i.e.

$$V'(\vec{r}) = \sum_{\vec{K}_\nu} V'_{K_\nu} \cos \vec{K}_\nu \cdot \vec{r}_c , \tag{69}$$

where

$$\vec{r}_c = \vec{r} - \vec{C}$$

is a position vector originated at some lattice site $\vec{C}$. Using this Fourier expansion, the potential energy integral becomes

$$\langle \psi_\alpha^s(\vec{A}) \mid V' \mid \phi_\beta^s(\vec{B}) \rangle = \sum_{\vec{K}_\nu} V'_{K_\nu} \langle \psi_\alpha^s(\vec{A}) \mid \cos \vec{K}_\nu \cdot \vec{r}_c \mid \phi_\beta^s(\vec{B}) \rangle , \tag{70}$$

where

$$\langle \psi_\alpha^s(\vec{A}) | \cos\vec{K}_\nu\cdot\vec{r}_C \, | \phi_\beta^s(\vec{B}) \rangle = \int \psi_\alpha^{*s}(\vec{r}_A) \cos\vec{K}_\nu\cdot\vec{r}_C \; \phi_\beta^s(\vec{r}_B) \, d\tau \, , \tag{71}$$

and where

$$\begin{aligned} \vec{A} &= [A_x, A_y, A_z] \, , \\ \vec{B} &= [B_x, B_y, B_z] \, , \\ \vec{C} &= [C_x, C_y, C_z] \, , \\ \vec{r} &= [x, y, z] \\ \vec{r}_A &= \vec{r} - \vec{A} \, , \\ \vec{r}_B &= \vec{r} - \vec{B} \, , \\ \vec{r}_C &= \vec{r} - \vec{C} \, . \end{aligned} \tag{72}$$

As will be shown, all necessary potential, overlap, and kinetic energy integrals can be obtained by performing the appropriate differentiations and summations of the single integral

$$\langle \psi_{1s}^s(\vec{A}) | \cos\vec{K}_\nu\cdot\vec{r}_C \, | \phi_{1s}^s(\vec{B}) \rangle = \int e^{-\alpha_1 r_A} \cos\vec{K}_\nu\cdot\vec{r}_C \; e^{-\alpha_2 r_B} \, d\tau \, . \tag{73}$$

In order to obtain a more manageable expression for this integral, first express the unnormalized Slater 1s orbitals $e^{-\alpha_1 r_A}$ and $e^{-\alpha_2 r_B}$ in laplace transforms [22]

$$\begin{aligned} e^{-\alpha_1 r_A} &= \frac{\alpha_1}{2\sqrt{\pi}} \int_0^\infty s_1^{-3/2} e^{-\alpha_1^2/4s_1} \, e^{-s_1 r_A^2} \, ds_1 \, , \\ e^{-\alpha_2 r_B} &= \frac{\alpha_2}{2\sqrt{\pi}} \int_0^\infty s_2^{-3/2} e^{-\alpha_2^2/4s_2} \, e^{-s_2 r_B^2} \, ds_2 \, , \end{aligned} \tag{74}$$

The integral $\langle \psi_{1s}^s(\vec{A}) | \cos\vec{K}_\nu\cdot\vec{r}_C \, | \phi_{1s}^s(\vec{B}) \rangle$ then becomes

$$\frac{\alpha_1 \alpha_2}{4\pi} \int_0^\infty (s_1 s_2)^{-3/2} \exp\{-[\frac{\alpha_1^2}{s_1} + \frac{\alpha_2^2}{s_2}]/4\} \{ \int e^{-s_1 r_A^2} e^{-s_2 r_B^2} \cos\vec{K}_\nu\cdot\vec{r}_C \, d\tau \} ds_1 ds_2 . \tag{75}$$

The spatial integral

$$\int e^{-s_1 r_A^2} e^{-s_2 r_B^2} \cos \vec{K}_\nu \cdot \vec{r}_c \, d\tau . \tag{76}$$

appearing in Eq. (75) can now be performed by using the fact that the product of two gaussians centered about points $\vec{A}$ and $\vec{B}$ respectively is proportional to a third gaussian centered about a point $\vec{D}$ along the line connecting $\vec{A}$ to $\vec{B}$, i.e.

$$\exp(-s_1 r_A^2) \exp(-s_2 r_B^2) = \exp\{-[s_1 s_2/(s_1+s_2)]\,\overline{AB}^2\} \exp\{-[s_1+s_2] r_D^2\} \tag{77}$$

where

$$\overline{AB}^2 = |\vec{B} - \vec{A}|^2 ,$$

$$r_D^2 = |\vec{r} - \vec{D}|^2 ,$$

$$\vec{D} = [D_x, D_y, D_z] ,$$

$$D_i = \frac{s_1 A_i + s_2 B_i}{s_1 + s_2} \qquad i = x, y, z .$$

Using this expression for the product of two gaussians, and rewriting $\cos \vec{K}_\nu \cdot \vec{r}_c$ as

$$\cos \vec{K}_\nu \cdot \vec{r}_c = \cos \vec{K}_\nu \cdot (\vec{r}_{CD} + \vec{r}_D), \tag{78}$$

$$= \cos \vec{K}_\nu \cdot \vec{r}_{CD} \cos \vec{K}_\nu \cdot \vec{r}_D - \sin \vec{K}_\nu \cdot \vec{r}_{CD} \sin \vec{K}_\nu \cdot \vec{r}_D ,$$

the spatial integral becomes

$$e^{-[s_1 s_2/(s_1+s_2)]\overline{AB}^2} \{\cos \vec{K}_\nu \cdot \vec{r}_{CD} \int e^{-(s_1+s_2) r_D^2} \cos \vec{K}_\nu \cdot \vec{r}_D \, d\tau - \sin \vec{K}_\nu \cdot \vec{r}_{CD} \int e^{-(s_1+s_2) r_D^2} \sin \vec{K}_\nu \cdot \vec{r}_D \, d\tau\} .$$

The two integrals in the above expression are easily evaluated, yielding

$$\int e^{-(s_1+s_2) r_D^2} \cos \vec{K}_\nu \cdot \vec{r}_D \, d\tau = [\pi/(s_1+s_2)]^{3/2} \exp\{-[K_\nu^2/(s_1+s_2)]/4\}$$

$$\int e^{-(s_1+s_2) r_D^2} \sin \vec{K}_\nu \cdot \vec{r}_D \, d\tau = 0 .$$

Using these results, the integral of Eq. (76) becomes

$$\int e^{-s_1 r_A^2}\, e^{-s_2 r_B^2} \cos \vec{K}_\nu \cdot \vec{r}_c \, d\tau = [\pi/(s_1+s_2)]^{3/2} \exp\{-[s_1 s_2/(s_1+s_2)]\overline{AB}^2\}$$
$$\times \exp\{-[K_\nu^2/(s_1+s_2)]/4\} \cos \vec{K}_\nu \cdot \vec{r}_{CD} ,$$

substituting this result into Eq. (75), the expression for $\langle \Psi_{1s}^{s}(\vec{A}) | \cos \vec{K}_\nu \cdot \vec{r}_c | \phi_{1s}^{s}(\vec{B}) \rangle$ becomes

$$\frac{\alpha_1 \alpha_2 \sqrt{\pi}}{4} \int_0^\infty (s_1 s_2)^{-3/2} (s_1+s_2)^{-3/2} \exp\{-[\alpha_1^2/s_1 + \alpha_2^2/s_2 + K_\nu^2/(s_1+s_2)]/4\}$$
$$\times \exp\{-[s_1 s_2/(s_1+s_2)]\overline{AB}^2\} \cos \vec{K}_\nu \cdot \vec{r}_{CD} \, ds_1 \, ds_2 . \qquad (79)$$

This integral can be simplified further by performing the change of variables

$$u = s_1/(s_1+s_2) ,$$
$$z = s_1 + s_2 . \qquad (80)$$

The Jacobian for this transformation is

$$\left| \frac{\partial(s_1, s_2)}{\partial(u, z)} \right| = z ,$$

and the integral $\langle \Psi_{1s}^{s}(\vec{A}) | \cos \vec{K}_\nu \cdot \vec{r}_c | \phi_{1s}^{s}(\vec{B}) \rangle$ becomes

$$\frac{\alpha_1 \alpha_2 2\sqrt{\pi}}{4} \int_0^1 \frac{\cos \vec{K}_\nu \cdot \vec{r}_{CD}}{[u(1-u)]^{3/2}} \, du \int_0^\infty z^{-7/2} e^{-fz} e^{-g/4z} \, dz \qquad (81)$$

where

$$f = u(1-u)\overline{AB}^2 ,$$
$$g = \alpha_1^2/u + \alpha_2^2/(1-u) + K_\nu^2 ,$$
$$\vec{r}_{CD} = \vec{D} - \vec{C} = \vec{r}_{CB} - u\vec{r}_{AB} .$$

The integral over z can be performed,[23] and the resulting expression for

$$\langle \Psi_{1s}^{s}(\vec{A}) \mid \cos\vec{K}_\nu \cdot \vec{r}_c \mid \phi_{1s}^{s}(\vec{B}) \rangle$$

is

$$2\pi\alpha_1\alpha_2\overline{AB}^3 \int_0^1 f\left[3(fg)^{-5/2}+3(fg)^{-2}+(fg)^{-3/2}\right]e^{-\sqrt{fg}}\cos\vec{K}_\nu\cdot\vec{r}_{CD}\,du\,. \qquad (82)$$

Thus the original three-center, three-dimensional integral over all space is reduced to a one-dimensional integral over finite limits of a well behaved integrand. This remaining integral is evaluated by numerical quadrature. Using the above expression for $\langle \Psi_{1s}^{s}(\vec{A}) \mid \cos\vec{K}_\nu \cdot \vec{r}_c \mid \phi_{1s}^{s}(\vec{B}) \rangle$ the corresponding potential integral $\langle \Psi_{1s}^{s}(\vec{A}) \mid V' \mid \phi_{1s}^{s}(\vec{B}) \rangle$ is easily determined by means of Eq. (70). Expressions for the other potential integrals can be obtained from Eq. (82) by performing the appropriate partial differentiations, viz.

$$\langle \Psi_{2s}^{s}(\vec{A}) \mid \cos\vec{K}_\nu \cdot \vec{r}_c \mid \phi_{1s}^{s}(\vec{B}) \rangle = -\frac{\partial}{\partial\alpha_1}\langle \Psi_{1s}^{s}(\vec{A}) \mid \cos\vec{K}_\nu \cdot \vec{r}_c \mid \phi_{1s}^{s}(\vec{B}) \rangle,$$

$$\langle \Psi_{2p_x}^{s}(\vec{A}) \mid \cos\vec{K}_\nu \cdot \vec{r}_c \mid \phi_{1s}^{s}(\vec{B}) \rangle = -\frac{\partial}{\partial\alpha_1}\left(\frac{1}{\alpha_1}\frac{\partial}{\partial A_x}\right)\langle \Psi_{1s}^{s}(\vec{A}) \mid \cos\vec{K}_\nu \cdot \vec{r}_c \mid \phi_{1s}^{s}(\vec{B}) \rangle,$$

$$\langle \Psi_{2s}^{s}(\vec{A}) \mid \cos\vec{K}_\nu \cdot \vec{r}_c \mid \phi_{2s}^{s}(\vec{B}) \rangle = -\frac{\partial}{\partial\alpha_2}\langle \Psi_{2s}^{s}(\vec{A}) \mid \cos\vec{K}_\nu \cdot \vec{r}_c \mid \phi_{1s}^{s}(\vec{B}) \rangle\,, \qquad (83)$$

$$\langle \Psi_{2p_x}^{s}(\vec{A}) \mid \cos\vec{K}_\nu \cdot \vec{r}_c \mid \phi_{2s}^{s}(\vec{B}) \rangle = -\frac{\partial}{\partial\alpha_2}\langle \Psi_{2p_x}^{s}(\vec{A}) \mid \cos\vec{K}_\nu \cdot \vec{r}_c \mid \phi_{1s}^{s}(\vec{B}) \rangle\,,$$

$$\langle \Psi_{2p_x}^{s}(\vec{A}) \mid \cos\vec{K}_\nu \cdot \vec{r}_c \mid \phi_{2p_x}^{s}(\vec{B}) \rangle = -\frac{\partial}{\partial\alpha_2}\left(\frac{1}{\alpha_2}\frac{\partial}{\partial B_x}\right)\langle \Psi_{2p_x}^{s}(\vec{A}) \mid \cos\vec{K}_\nu \cdot \vec{r}_c \mid \phi_{1s}^{s}(\vec{B}) \rangle\,,$$

$$\langle \Psi_{2p_x}^{s}(\vec{A}) \mid \cos\vec{K}_\nu \cdot \vec{r}_c \mid \phi_{2p_y}^{s}(\vec{B}) \rangle = -\frac{\partial}{\partial\alpha_2}\left(\frac{1}{\alpha_2}\frac{\partial}{\partial B_y}\right)\langle \Psi_{2p_x}^{s}(\vec{A}) \mid \cos\vec{K}_\nu \cdot \vec{r}_c \mid \phi_{1s}^{s}(\vec{B}) \rangle\,,$$

where $\Psi_\alpha^s(\vec{A})$ and $\phi_\alpha^s(\vec{B})$ are the unnormalized Slater-type orbitals

$$\Psi_{1s}^{s}(\vec{A}) = e^{-\alpha_1 r_A} \qquad \phi_{1s}^{s}(\vec{B}) = e^{-\alpha_2 r_B}$$

$$\Psi_{2s}^{s}(\vec{A}) = r_A e^{-\alpha_1 r_A} \qquad \phi_{2s}^{s}(\vec{B}) = r_B e^{-\alpha_2 r_B}$$

$$\Psi_{2p_x}^{s}(\vec{A}) = x_A e^{-\alpha_1 r_A} \qquad \phi_{2p_x}^{s}(\vec{B}) = x_B e^{-\alpha_2 r_B}\,,$$

etc. centered about points $\vec{A}$ and $\vec{B}$ respectively. In general, the integrals of

$\cos\vec{K}_\nu\cdot\vec{r}_A$ may be written in the form

$$\langle\Psi_\alpha^s(\vec{A})|\cos\vec{K}_\nu\cdot\vec{r}_A|\phi_\beta^s(\vec{B})\rangle = 2\pi\sum_i \beta_i \int_0^1 \gamma_i(u)\Big[\sum_{n=0}^{7}\mu_{i,n}(fg)^{-(9-n)/2}\Big] \quad (84)$$
$$\times\ e^{-\sqrt{fg}}\{\xi_{i,1}\cos[(1-u)\vec{K}_\nu\cdot\vec{r}_{AB}] + \xi_{i,2}\sin[(1-u)\vec{K}_\nu\cdot\vec{r}_{AB}]\}\,du\,,$$

where the summation over i may include one, two, three, or four terms depending on the orbitals Ψ_α^s and ϕ_β^s. The coefficients for Eq. (84) corresponding to the various integrals of $\cos\vec{K}_\nu\cdot\vec{r}_A$ are given in Table 6. From these integrals, all the necessary potential integrals can be constructed by means of Eq. (70).

B. Overlap Integrals.

The overlap integrals $\langle\Psi_\alpha^s(\vec{A})|\ \phi_\beta^s(\vec{B})\rangle$ of two unnormalized Slater-type orbitals can be obtained from the corresponding integrals

$$\langle\Psi_\alpha^s(\vec{A})|\cos\vec{K}_\nu\cdot\vec{r}_c|\phi_\beta^s(\vec{B})\rangle$$

by merely setting $\vec{K}_\nu$ equal to zero. The resulting integrals can be expressed as

$$\langle\Psi_\alpha^s(\vec{A})|\phi_\beta^s(\vec{B})\rangle = 2\pi\sum_i \zeta_i \int_0^1 \eta_i(u)\Big[\sum_{n=0}^{7}\lambda_{i,n}(fG)^{-(9-n)/2}\Big]e^{-\sqrt{fG}}\,du\,, \quad (85)$$

where

$$G = \alpha_1^2/u + \alpha_2^2/(1-u).$$

Table 7 lists all the coefficients for the various overlap integrals.

C. Kinetic Energy Integrals.

In order to obtain simple expressions for the kinetic energy integrals $\langle\Psi_\alpha^s(\vec{A})|-\frac{1}{2}\nabla^2|\phi_\beta^s(\vec{B})\rangle$, examine the factor in the integrand

$$\nabla^2\phi_\beta^s(\vec{r}_B) = \Big(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\Big)\phi_\beta^s(x_B,y_B,z_B) \quad (86)$$

where

$$x_B = x - B_x \qquad y_B = y - B_y \qquad z_B = z - B_z\,.$$

The laplacian is invariant under translation of the coordinate system and hence,

$$\nabla^2 \phi_\beta^s(\vec{r}_B) = \left(\frac{\partial^2}{\partial x_B^2} + \frac{\partial^2}{\partial y_B^2} + \frac{\partial^2}{\partial z_B^2}\right) \phi_\beta^s(x_B, y_B, z_B). \tag{87}$$

Due to the symmetrical relationship of x_B and B_x in $\phi_\beta^s(x_B, y_B, z_B)$ one obtains the relation

$$\frac{\partial \phi^s(\vec{r}_B)}{\partial B_x} = \frac{\partial \phi^s(\vec{r}_B)}{\partial x_B} \frac{\partial x_B}{\partial B_x} = - \frac{\partial \phi^s(\vec{r}_B)}{\partial x_B}, \tag{88}$$

and similar relations for y and z. Hence,

$$\nabla^2 \phi_\beta^s(\vec{r}_B) = \nabla_B^2 \phi_\beta^s(\vec{r}_B), \tag{89}$$

where

$$\nabla_B^2 = \frac{\partial^2}{\partial B_x^2} + \frac{\partial^2}{\partial B_y^2} + \frac{\partial^2}{\partial B_z^2}.$$

Using the result of Eq. (89), it is seen that each kinetic energy integral can be obtained by applying the operator $-\frac{1}{2}\nabla_B^2$ to the corresponding overlap integral, i.e.

$$\langle \Psi_\alpha^s(\vec{A}) | -\frac{1}{2}\nabla^2 | \phi_\beta^s(\vec{B}) \rangle = -\frac{1}{2}\nabla_B^2 \langle \Psi_\alpha^s(\vec{A}) | \phi_\beta^s(\vec{B}) \rangle. \tag{90}$$

The kinetic energy integrals which result from performing these differentiations can be expressed in the form

$$\langle \Psi_\alpha^s(\vec{A}) | -\frac{1}{2}\nabla^2 | \phi_\beta^s(\vec{B}) \rangle = \pi \sum_i \omega_i \int_0^1 \eta_i(u) \left[\sum_{n=0}^{7} \rho_{i,n} (fG)^{-(7-n)/2} \right] e^{-\sqrt{fG}}\, du \tag{91}$$

and the coefficients corresponding to the different choices for Ψ_α^s and ϕ_β^s are given in Table 8.

In order to determine the accuracy and convergence of these expressions, a number of simplified test integrals were performed and the answers were

compared with Kotani's Tables. [18] The results of these test integrals is given in the appendix. These results show that both convergence and accuracy are excellent.

Table 6
Coefficients for $\langle \psi^s(\vec{A}) | \cos K_\nu \cdot r_A | \phi^s(\vec{B}) \rangle$

ψ^s	ϕ^s	i	β_i	$\gamma_i(u)$	$\mu_{i,0}$	$\mu_{i,1}$	$\mu_{i,2}$	$\mu_{i,3}$	$\mu_{i,4}$	$\mu_{i,5}$	$\mu_{i,6}$	$\mu_{i,7}$	$\xi_{i,1}$	$\xi_{i,2}$
1s	1s	1	$\alpha_1 \alpha_2 \overline{AB}^3$	f	0	0	0	0	3	3	1	0	1	0
2s	1s	1	$\alpha_1^2 \alpha_2 \overline{AB}^3$	f^2/u	0	0	15	15	6	1	0	0	1	0
		2	$-\alpha_2 \overline{AB}^3$	f	0	0	0	0	3	3	1	0	1	0
$2p_x$	1s	1	$-\alpha_1 \alpha_2 (K_\nu)_x \overline{AB}^3$	f^2	0	0	15	15	6	1	0	0	0	1
		2	$\alpha_1 \alpha_2 \overline{AB}\ \overline{AB}_x$	f^2/u	0	0	0	0	3	3	1	0	1	0
2s	2s	1	$\alpha_1^2 \alpha_2^2 \overline{AB}^5$	f^2	105	105	45	10	1	0	0	0	1	0
		2	$\overline{AB}^3 K_\nu^2$	f^2	0	0	15	15	6	1	0	0	1	0
		3	$-\overline{AB}^3$	f	0	0	0	0	12	12	5	1	1	0
$2p_x$	2s	1	$-\alpha_1 \alpha_2^2 (K_\nu)_x \overline{AB}^3$	$f^3/(1-u)$	105	105	45	10	1	0	0	0	0	1
		2	$\alpha_1 \alpha_2^2 \overline{AB}_x \overline{AB}^3$	f^2	0	0	15	15	6	1	0	0	1	0
		3	$\alpha_1 (K_\nu)_x \overline{AB}^3$	f^2	0	0	15	15	6	1	0	0	0	1
		4	$-\alpha_1 \overline{AB}\ \overline{AB}_x$	f^2/u	0	0	0	0	3	3	1	0	1	0

ψ^s	ϕ^s	i	β_i	$\Upsilon_i(\upsilon)$	$\mu_{i,0}$	$\mu_{i,1}$	$\mu_{i,2}$	$\mu_{i,3}$	$\mu_{i,4}$	$\mu_{i,5}$	$\mu_{i,6}$	$\mu_{i,7}$	$\xi_{i,1}$	$\xi_{i,2}$
$2p_x$	$2p_x$	1	$-\alpha_1\alpha_2(K_\nu)_x^2\overline{AB}^3$	f^3	105	105	45	10	1	0	0	0	1	0
		2	$\alpha_1\alpha_2\overline{AB}^3$	f^2	0	0	15	15	6	1	0	0	1	0
		3	$\alpha_1\alpha_2(K_\nu)_x\overline{AB}^3\overline{AB}_x$	$(2\upsilon-1)f^2$	0	0	15	15	6	1	0	0	0	1
		4	$-\alpha_1\alpha_2\overline{AB}\,\overline{AB}_x^{\,2}$	f^2	0	0	0	0	3	3	1	0	1	0
$2p_x$	$2p_y$	1	$-\alpha_1\alpha_2\overline{AB}^3(K_\nu)_x(K_\nu)_y$	f^3	105	105	45	10	1	0	0	0	1	0
		2	$\alpha_1\alpha_2\overline{AB}^3$	$\{[(K_\nu)_x\overline{AB}_y$	0	0	15	15	6	1	0	0	0	1
				$+(K_\nu)_y\overline{AB}_x]\upsilon$										
				$-(K_\nu)_y\overline{AB}_x]f^2$										
		3	$-\alpha_1\alpha_2\overline{AB}\,\overline{AB}_x\overline{AB}_y$	f^2	0	0	0	0	3	3	1	0	1	0

Table 7
Coefficients for $\langle \Psi^s(\vec{A}) | \phi^s(\vec{B}) \rangle$

Ψ^s	ϕ^s	i	ζ_i	$\eta_i(v)$	$\lambda_{i,0}$	$\lambda_{i,1}$	$\lambda_{i,2}$	$\lambda_{i,3}$	$\lambda_{i,4}$	$\lambda_{i,5}$	$\lambda_{i,6}$	$\lambda_{i,7}$
1s	1s	1	$\alpha_1 \alpha_2 \overline{AB}^3$	f	0	0	0	0	3	3	1	0
2s	1s	1	$\alpha_1^2 \alpha_2 \overline{AB}^3$	f^2/v	0	0	15	15	6	1	0	0
		2	$-\alpha_2 \overline{AB}^3$	f	0	0	0	0	3	3	1	0
$2p_x$	1s	1	$\alpha_1 \alpha_2 \overline{AB}\ \overline{AB}_x$	f^2/v	0	0	0	0	3	3	1	0
2s	2s	1	$\alpha_1^2 \alpha_2^2 \overline{AB}^5$	f^2	105	105	45	10	1	0	0	0
		2	$-\overline{AB}^3$	f	0	0	0	0	12	12	5	1
$2p_x$	2s	1	$\alpha_1 \alpha_2^2 \overline{AB}^3 \overline{AB}_x$	f^2	0	0	15	15	6	1	0	0
		2	$-\alpha_1 \overline{AB}\ \overline{AB}_x$	f^2/v	0	0	0	0	3	3	1	0
$2p_x$	$2p_x$	1	$\alpha_1 \alpha_2 \overline{AB}^3$	f^2	0	0	15	15	6	1	0	0
		2	$-\alpha_1 \alpha_2 \overline{AB}\ \overline{AB}_x^2$	f^2	0	0	0	0	3	3	1	0
$2p_x$	$2p_y$	1	$-\alpha_1 \alpha_2 \overline{AB}\ \overline{AB}_x \overline{AB}_y$	f^2	0	0	0	0	3	3	1	0

Table 8
Coefficients for $\langle \Psi^s(\vec{A}) | -\frac{1}{2}\nabla^2 | \phi^s(\vec{B}) \rangle$

Ψ^s	ϕ^s	i	ω_i	$\eta_i(u)$	$\rho_{i,0}$	$\rho_{i,1}$	$\rho_{i,2}$	$\rho_{i,3}$	$\rho_{i,4}$	$\rho_{i,5}$	$\rho_{i,6}$	$\rho_{i,7}$
1s	1s	1	$\alpha_1\alpha_2\overline{AB}$	f	0	0	0	0	3	3	-1	0
2s	1s	1	$\alpha_1^2\alpha_2\overline{AB}$	f^2/u	0	0	9	9	2	-1	0	0
		2	$-\alpha_2\overline{AB}$	f	0	0	0	0	3	3	-1	0
$2p_x$	1s	1	$\alpha_1\alpha_2\overline{AB}_x/\overline{AB}$	f^2/u	0	0	0	0	5	5	-1	0
2s	2s	1	$\alpha_1^2\alpha_2^2\overline{AB}^3$	f^2	45	45	15	0	-1	0	0	0
		2	$-\overline{AB}$	f	0	0	0	0	6	6	3	-1
$2p_x$	2s	1	$\alpha_1\alpha_2^2\overline{AB}_x\overline{AB}$	f^2	0	0	15	15	4	-1	0	0
		2	$-\alpha_1\overline{AB}_x/\overline{AB}$	f^2/u	0	0	0	0	5	5	-1	0
$2p_x$	$2p_x$	1	$\alpha_1\alpha_2\overline{AB}$	f^2	0	0	15	15	4	-1	0	0
		2	$-\alpha_1\alpha_2\overline{AB}_x^2/\overline{AB}$	f^2	0	0	0	0	7	7	-1	0
$2p_x$	$2p_y$	1	$-\alpha_1\alpha_2\overline{AB}_x\overline{AB}_y/\overline{AB}$	f^2	0	0	0	0	7	7	-1	0

CHAPTER VII

RESULTS AND CONCLUSIONS

The calculations of the conduction band of lithium were performed for the two choices of the fundamental lattice constant $a_0 = 6.65$ and 6.5183 au. In both cases, all summations involved in calculating the matrix elements were carried to convergence.

For $a_0 = 6.65$ au, the conduction band was calculated along the three major lines of symmetry [100], [110], [111] and along the face diagonal G given by $k_z = 0$, $k_x + k_y = 2\pi/a_0$. The results of these calculations are given in Table 9. Where available, the results of Ham's calculations by the method of Green's Function are presented for comparison. As can be seen, the agreement between these calculations is quite good. To exhibit the spherical nature of the conduction band around the point $\vec{k} = 0$, the three major lines of symmetry are plotted together in Fig. (2).

For $a_0 = 6.5183$ au, the conduction band was calculated along the symmetry lines [100], [110], [111], [221], [310], [311] and along the two face diagonals G and D given by $k_z = 0$, $k_x + k_y = 2\pi/a_0$, and by $k_y = k_z =$

π/a_0, $|\ k_x\ | < \pi/a_0$ respectively. The results of these calculations are given in Table 10. The results of calculations by Schlosser and Marcus and by Brown and Krumhansl using the methods of composite waves and modified plane waves respectively are presented in Table 10 for comparison with the results of tight-binding and again the agreement is seen to be quite good.

In the calculations of Schlosser and Marcus and of Brown and Krumhansl, $\bar{V}$ was taken to be -0.3314 au whereas the $\bar{V}$ used in the tight-binding calculation was -0.3248 au for both $a_0 = 6.65$ and 6.5183 au. This difference in the choice of $\bar{V}$ does not change the potential within the inscribed spheres but results in a higher barrier between the inscribed spheres in the tight-binding calculation. The potential barrier between the spheres is 0.0066 au higher in the tight-binding calculation than it is in the calculations of composite waves and modified plane waves. Thus if H_0 is the one-electron Hamiltonian used in the present tight-binding calculation and if H is the Hamiltonian used by Schlosser and Marcus and by Brown and Krumhansl, then

$$H = H_0 + H' \ , \tag{92}$$

where H' is equal to zero within the inscribed spheres and equal to -0.0066 au between the inscribed spheres. Using the expression of Eq. (92), a rough perturbation-like calculation can be performed to estimate the effect that this difference in potential has on the energy band calculations. If the energy associated with H_0 is designated as $E_0(\vec{K})$ and that associated with H is designated as $E(\vec{K})$, then to first order

$$E(\vec{k}) = E_0(\vec{k}) + E'(\vec{k}) \ , \tag{93}$$

where

$$E'(\vec{k}) = \frac{\int \psi^*(\vec{k},\vec{r})\, H' \psi\ (\vec{k},\vec{r})\, d\tau}{\int \psi^*(\vec{k},\vec{r})\ \psi\ (\vec{k},\vec{r})\, d\tau} \quad .$$

Using the fact that H' is zero within the inscribed spheres, the expression for $E'(\vec{k})$ becomes

$$E'(\vec{k}) = H' \int_{\Delta\Omega} \psi^*(\vec{k},\vec{r})\, \psi\ (\vec{k},\vec{r})\, d\tau \Big/ \int_{\Omega} \psi^*(\vec{k},\vec{r})\, \psi\ (\vec{k},\vec{r})\, d\tau \qquad (94)$$

where

$$\int_{\Omega} \psi^*(\vec{k},\vec{r})\, \psi\ (\vec{k},\vec{r})\, d\tau,$$

is the integral of $\psi^*(\vec{k},\vec{r})\,\psi\ (\vec{k},\vec{r})$ over the Wigner-Seitz cell and where

$$\int_{\Delta\Omega} \psi^*(\vec{k},\vec{r})\, \psi\ (\vec{k},\vec{r})\, d\tau\ ,$$

is the integral of $\psi^*(\vec{k},\vec{r})\,\psi\ (\vec{k},\vec{r})$ over that region of the Wigner-Seitz cell which is exterior to the inscribed sphere. For the lower portion of the conduction band, the charge density is roughly constant in space and

$$\frac{\int_{\Delta\Omega} \psi^*(\vec{k},\vec{r})\, \psi\ (\vec{k},\vec{r})\, d\tau}{\int_{\Omega} \psi^*(\vec{k},\vec{r})\, \psi\ (\vec{k},\vec{r})\, d\tau} \approx \frac{\Delta\Omega}{\Omega} = 0.320. \qquad (95)$$

Using this expression in Eq. (93) yields

$$E' \approx -0.002\text{au} = -0.004\ R_y\ . \qquad (96)$$

Thus the effect of this difference in the choice of $\bar{V}$ is negligible and in fact Eqs. (93) and (96) show that when this difference is accounted for, the agreement is actually improved.

For points of high symmetry, the secular equation factorizes into smaller blocks due to the transformation requirements of the group of the wave vector. For example, at the Γ point only the mixing between 1s and 2s Bloch functions need be considered, whereas along the Δ line of [100] symmetry,

the secular equation is a 3x3 one with 1s, 2s, and $2p_x$ basis functions. For an arbitrary point in the k-space, the complete 5x5 secular equation must be solved. However, once all the basic integrals have been evaluated, the energy for any point in the Brillouin zone can be obtained as readily as that for a point of high symmetry.

To examine the effect of the 1s core on the band structure, the energy of the Γ point was calculated using two separate approximations. The first of these is to completely ignore the 1s Bloch function and gives $E = -0.896$ Ry. The second is to leave out the 1s basis function and orthogonalize the 2s Bloch sum to the 1s one, i.e.

$$b_{2s}^{orth}(\vec{k}=0, \vec{r}) = b_{2s}(\vec{k}=0, \vec{r}) + q b_{1s}(\vec{k}=0, \vec{r}). \qquad (97)$$

This gives $E = -0.675$ Ry in very close agreement with -0.672 Ry obtained by including the 1s function. Since there is no mixing at the Γ point between basis functions of s and p symmetry, the wave function at the Γ point corresponding to this stage of approximation is simply $b_{2s}^{orth}(\vec{k}=0, \vec{r})$. To carry this scheme of approximation outside the Γ point, one finds that the k-dependence of the 1s-2s and 1s-2p mixing coefficients causes considerable complication in the computations. In place of the properly orthogonalized 2s Bloch function b_{2s}^{orth}, the Bloch sum

$$b_{2s}'(\vec{k}, \vec{r}) = [N \Omega_{2s}(\vec{k})]^{-1/2} \sum_{\nu} e^{i\vec{k}\cdot\vec{R}_\nu} [\phi_{2s}(\vec{r}-\vec{R}_\nu) + q\, \phi_{1s}(\vec{r}-\vec{R}_\nu)] \qquad (98)$$

was used where q has the same value as that appearing in Eq. (97). The b_{2s}' and the three b_{2p} functions then form the basis of a 4x4 secular equation which yields an alternative set of energy values as shown in Table II. Near the Γ

point the deviations of this set of energies from the corresponding solutions of the 5x5 secular equation increase with $\vec{k}$ since b_{2s}' is not orthogonal to b_{1s} except for $\vec{k} = 0$. Although one may expect to obtain better energy values using the properly orthogonalized 2s Bloch functions, the numerical computation is much simpler with $b_{2s}'(\vec{k}, \vec{r})$ which proves to be more useful from a practical standpoint. As one approaches the edges of the Brillouin zone, the band functions become more p-like and better agreements are thus found between the energy solutions of the 4x4 and of the 5x5 secular equations. Included in the next to the last column of Table 11, are the energy solutions of the 4x4 secular equation with b_{2s} in place of b_{2s}' thereby neglecting the 1s core completely. The results of this drastic approximation are rather poor except near the edge of the Brillouin zone where the wave functions have primarily p-characters.

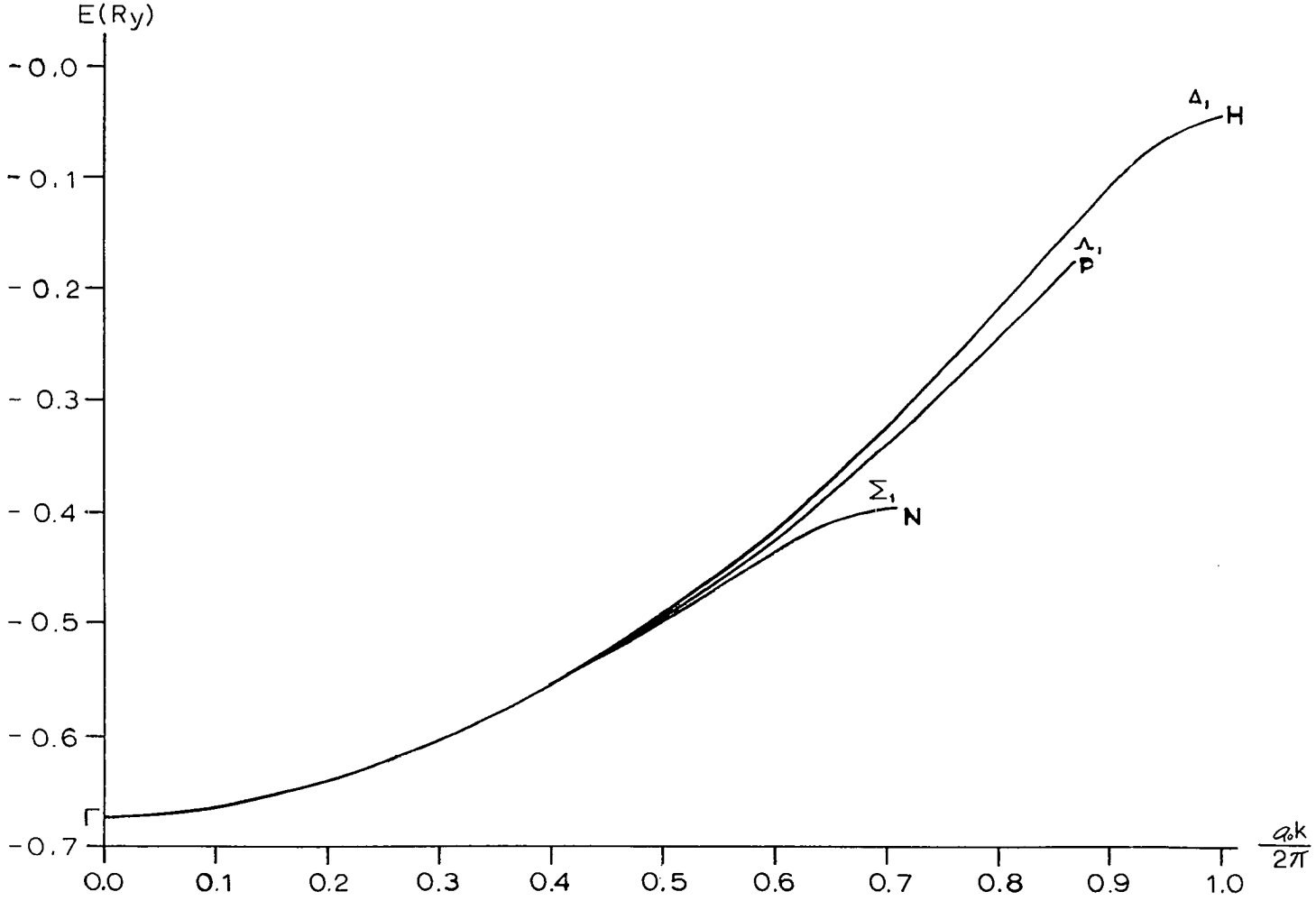
To investigate the importance of the b_{2p} in determining the band structure, the 2x2 secular equation formed by neglecting the b_{2p_x}, b_{2p_y}, b_{2p_z} basis functions was computed at various points in the Brillouin zone. The results of these calculations are given in the last column of Table 11. As would be expected, these results show that the b_{2p} dominate in the outer regions of the Brillouin zone but have little effect on the conduction band in the region of the Γ point.

These results indicate that the tight-binding method is applicable to a much larger family of crystals than is currently believed. Indeed, even when the overlap between neighboring atomic orbitals is extremely large, as is the case in lithium, the method of tight-binding can still be expected to yield accurate

energies and extremely simple wave functions. Furthermore, unlike some purely mathematical methods, the method of tight-binding lends itself easily to physical interpretation and provides a great deal of physical insight into the problem of solids in general.

The wave function for $\vec{k} = 2\pi/a_0\,(1,0,0)$, H_1-point, is given in Fig. (3) along the x axis and along the line $x = y = z$ for lattice constant $a_0 = 6.5183$au. Fig. (3) demonstrates the strong angular dependence of the wave function which is characteristic of p-symmetry.

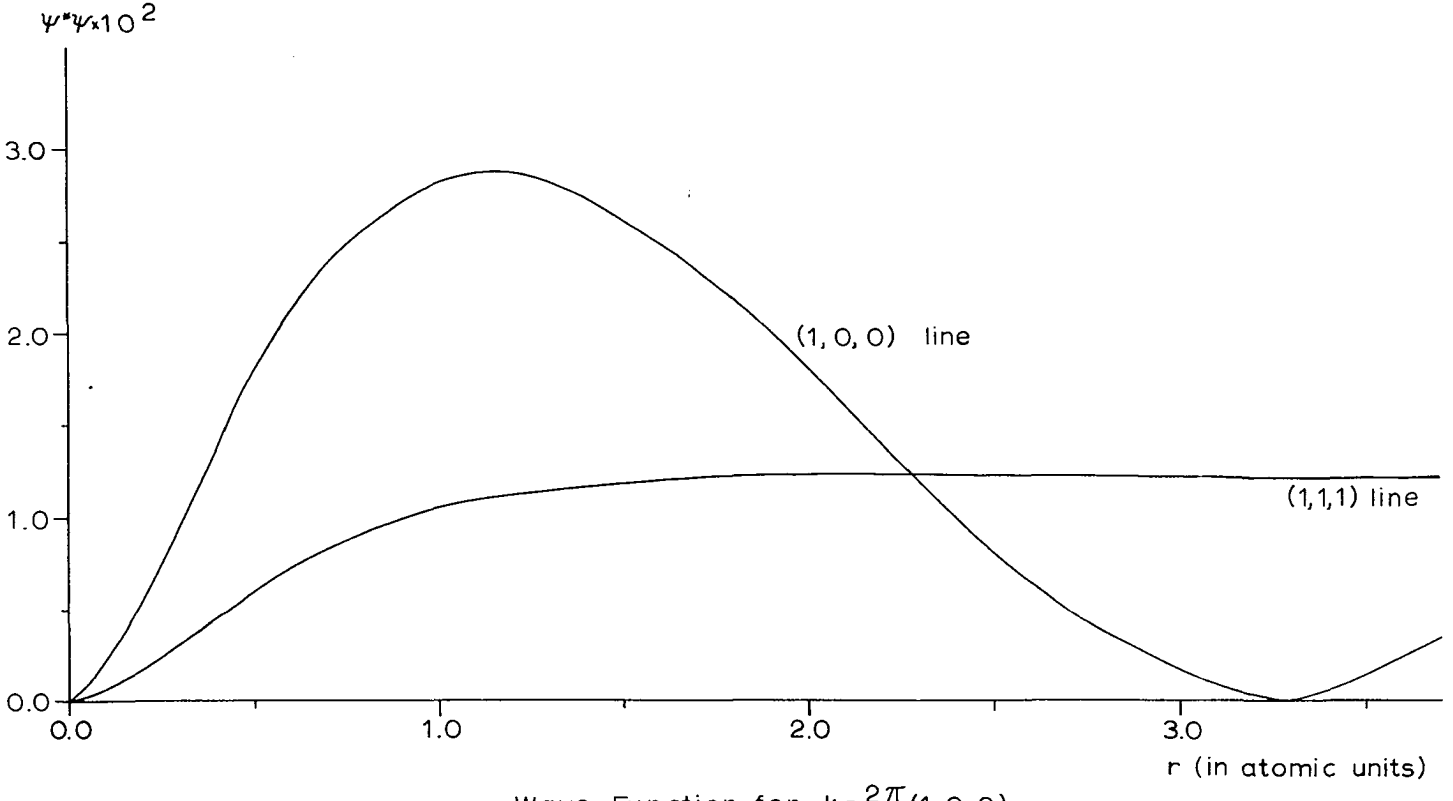
Due to the lack of direct experimental measurements of the energy band structure in the region investigated, comparison with experiment was not possible. In order to make such comparisons, band gap, etc., the higher energy bands would also have to be obtained. As mentioned previously, investigation of the higher bands is not feasible with such a limited number of basis functions. The present method of calculation is, at present, being applied to the group IV compounds with a larger number of basis functions and it is hoped that more direct comparison with experiment will be possible.



Structure of Three Major Symmetry Lines

(a_0 = 6.65 au)

Figure 2



Wave Function for $k=\frac{2\pi}{a_o}(1, 0, 0)$

Figure 3

Table 9

Comparison of the energies (in Rydberg's) of the conduction band of lithium calculated by the tight-binding method and by the method of Green's Functions. (a_0=6.65au)

$\frac{a_0 k_x}{2\pi}$	Energies	
	Tight-binding	Green's Functions[a]
[100] Δ_1		
0.0000	-0.674	-0.681
0.0500	-0.672	
0.1000	-0.666	
0.1500	-0.657	
0.2000	-0.645	
0.2500	-0.629	-0.640
0.3000	-0.610	
0.3500	-0.587	
0.4000	-0.562	
0.4500	-0.533	
0.5000	-0.500	-0.512
0.5500	-0.465	
0.6000	-0.426	
0.6250	-0.407	-0.414
0.6500	-0.384	
0.7000	-0.339	
0.7500	-0.290	-0.294
0.8000	-0.236	
0.8500	-0.178	
0.9000	-0.121	
0.9500	-0.080	
1.0000	-0.065	-0.061
[110] Σ_1		
0.1000	-0.659	
0.2000	-0.617	
0.2500	-0.587	-0.598
0.3000	-0.550	
0.3750	-0.395	-0.497
0.4000	-0.462	
0.5000	-0.399	-0.411

[a]See reference 9.

$\frac{a_0 k_x}{2\pi}$	Energies	
	Tight-binding	Green's Functions[a]
[111] Λ_1		
0.1000	-0.652	
0.1250	-0.641	-0.651
0.2000	-0.590	
0.2500	-0.545	-0.556
0.3000	-0.490	
0.3125	-0.478	-0.486
0.3750	-0.395	-0.400
0.4000	-0.355	
0.5000	-0.190	-0.191
Face Diagonal G		
1.000	-0.065	
0.900	-0.137	
0.800	-0.252	
0.700	-0.334	
0.600	-0.383	
0.500	-0.411	

Table 10

Comparison of the energies (in Rydberg's) of the conduction band of lithium calculated by the tight-binding method and by the methods of modified plane waves and the method of composite waves (a_0=6.5183).

$\frac{a_0 k_x}{2\pi}$	Modified[a] Plane Waves	Composite[b] Waves	Tight-binding 5x5 secular equation
[100] Δ_1			
0.00	-0.683	-0.683	-0.672
0.05			-0.670
0.15			-0.656
0.20	-0.652	-0.656	-0.643
0.25			-0.627
0.35			-0.584
0.45			-0.527
0.50	-0.495	-0.510	-0.495
0.55			-0.458
0.65			-0.375
0.75			-0.278
0.80		-0.233	-0.223
0.85			-0.164
0.90		-0.119	-0.106
0.95			-0.061
0.96		-0.061	-0.055
1.00		-0.046	-0.044
[110] Σ_1			
0.05			-0.668
0.10		-0.669	-0.657
0.15			-0.639
0.25			-0.583
0.30		-0.562	-0.545
0.35			-0.503
0.45			-0.414
0.50		-0.410	-0.393
[111] Λ_1			
0.05			-0.667
0.10		-0.663	-0.650

[a]See reference 11.

[b]See reference 10.

$\frac{a_0 k_x}{2\pi}$	Modified[a] Plane Waves	Composite[b] Waves	Tight-binding 5x5 secular equation
0.15			-0.623
0.20	-0.590		-0.587
0.25			-0.540
0.30		-0.500	-0.484
0.35			-0.420
0.40	-0.336	-0.358	-0.346
0.45			-0.265
0.50	-0.175	-0.184	-0.177
[221]			
0.20		-0.620	-0.607
0.35		-0.496	-0.482
0.50		-0.353	-0.340
[310]			
0.300		-0.615	-0.600
0.525		-0.474	-0.458
0.750		-0.294	-0.288
[311]			
0.300		-0.608	-0.593
0.525		-0.453	-0.439
Face Diagonal G			
1.000			-0.044
0.900			-0.122
0.800			-0.242
0.700			-0.326
0.600			-0.377
0.500			-0.393
Face Diagonal D			
0.000			-0.393
0.100			-0.385
0.200			-0.360
0.300			-0.317
0.400			-0.257
0.500			-0.177

Table 11

Effects of various approximations on the structure of the conduction band of lithium for $a_0 = 6.5183$.

$\frac{a_0 k_x}{2\pi}$	Tight-binding 5x5 secular equation	Simplified Tight-binding 4x4 Using b_{2s}	4x4 Using b_{2s}	2x2 Using b_{1s} and b_{2s}
$[100]\Delta_1$				
0.0	-0.672	-0.676	-0.896	-0.672
0.2	-0.643	-0.642	-0.556	-0.642
0.5	-0.495	-0.487	-0.452	-0.472
0.8	-0.223	-0.221	-0.219	+0.185
0.9	-0.106	-0.106	-0.106	
1.0	-0.044	-0.044	-0.044	
$[110]\Sigma_1$				
0.1	-0.657	-0.657	-0.508	-0.657
0.3	-0.545	-0.537	-0.451	-0.529
0.5	-0.393	-0.393	-0.393	-0.160
$[111]\Lambda_1$				
0.1	-0.650	-0.649	-0.536	-0.649
0.2	-0.587	-0.582	-0.509	-0.580
0.3	-0.484	-0.473	-0.413	-0.446
0.4	-0.346	-0.342	-0.324	-0.132
0.5	-0.177	-0.177	-0.177	+0.268

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APPENDIX I

As is seen in Chapter VI, the multicenter integrals of overlap, kinetic energy, and potential energy can be reduced to a sum of one-dimensional integrals over finite limits zero to one as given in Tables 6 through 8. These one-dimensional integrals are then evaluated by numerical quadrature. The technique of integration chosen is that of Gaussian quadrature. To check the accuracy of this formulation and the associated computer programs, a number of test integrals of overlap, kinetic energy, and potential energy were computed for unnormalized Slater-type orbitals. The results of these tests are presented in the first three sections of this appendix. The fourth and last section gives all the multicenter-integrals necessary for setting up the secular equation of any point in the Brillouin zone of lithium.

A. Tests of Overlap Integrals

In these tests, the overlap integrals $\langle \psi^S_\mu (A) | \phi^S_\nu (B) \rangle$ were calculated from Table 7 for unnormalized Slater-type orbitals $\langle \psi^S_\mu (A)$ and $\phi^S_\nu (B) \rangle$ defined by Eq. (83) and situated at points A and B respectively. The results of calculations using 16-point quadrature are given in Table A-1 along with a

comparison with the results of Kotani's tables.[11]

B. Tests of Kinetic Energy Integrals

Here the kinetic energy integral formulation given in Table 8 was tested by using 16-point quadrature (except for $\mu = 2p_x$, $\nu = 2p_y$ where 40-point quadrature was used) and the resulting integrals are given in Table A-II along with comparisons with Kotani's tables.

C. Tests of Potential Energy Integrals

The formulation, based on Table 7, of the potential energy integrals $\langle \Psi^S_\mu(\vec{A}) | V' | \phi^S_\nu(\vec{B}) \rangle$ is difficult to test due to the fact that there are no tables of integrals to compare with. This difficulty can be overcome by choosing a very special form for $V'(r)$ and by choosing the parameters $\vec{A}$, $\vec{B}$, α_1, and α_2 very carefully. Namely, let $V'(r)$ be unity within each inscribed sphere and zero between the inscribed spheres, choose $\vec{A}$ and $\vec{B}$ to lie close together within the same inscribed sphere, and let α_1 and α_2 be so large that $\Psi^S_\mu(A)$ and $\phi^S_\nu(B)$ are essentially zero outside this sphere. Under these stringent requirements, the integral $\langle \Psi^S_\mu(\vec{A}) | V' | \phi^S_\nu(B) \rangle$ can be closely approximated by the overlap integral $\langle \Psi^S_\mu(\vec{A}) | \phi^S_\nu(\vec{B}) \rangle$. Table A-III presents the results of such a calculation and compares the results with the corresponding overlap integral. Considering the approximations involved, the agreement is excellent.

D. Integrals for Lithium

Tables A-IV through A-XIII give the multicenter integrals

$$\langle \psi_\alpha (\vec{A} = 0) \mid \psi_\beta (\vec{B} = \vec{R}_\nu) \rangle,$$

$$\langle \psi_\alpha (\vec{A} = 0) \mid -\frac{1}{2} \nabla^2 \mid \psi_\beta (\vec{B} = \vec{R}_\nu) \rangle,$$

$$\langle \psi_\alpha (\vec{A} = 0) \mid V' \mid \psi_\beta (\vec{B} = \vec{R}_\nu) \rangle$$

for all values of $\vec{R}_\nu$ for which the integrals are appreciable. Here the functions are not the unnormalized Slater-type orbitals but rather are the curve fits of the Hartree-Fock solutions for the free lithium atom as given in Eq. (55). The calculation of these integrals is a basic necessity for any tight-binding calculation and comprises over 99% of the labor involved in an accurate tight-binding calculation. Using these tables and the results of Chapter V, one can easily find the energy and wave function of any desired point in the Brillouin zone.

Of the integrals involving two 1s orbitals centered at points $\vec{A}$ and $\vec{B}$, the only integrals of appreciable magnitude are those for which $\vec{A} = \vec{B}$. For $a_0 = 6.65$ au these are

$$\langle \psi_{1s}(\vec{0}) \mid \psi_{1s}(\vec{0}) \rangle = +1.00013,$$

$$\langle \psi_{1s}(\vec{0}) \mid -\frac{1}{2} \nabla^2 \mid \psi_{1s}(\vec{0}) \rangle = +3.6104,$$

$$\langle \psi_{1s}(\vec{0}) \mid V' \mid \psi_{1s}(\vec{0}) \rangle = -5.1522,$$

and for $a_0 = 6.5183$ au

$$\langle \psi_{1s}(\vec{0}) \mid \psi_{1s}(\vec{0}) \rangle = +1.00013,$$

$$\langle \psi_{1s}(\vec{0}) \mid -\frac{1}{2} \nabla^2 \mid \psi_{1s}(\vec{0}) \rangle = +3.6104,$$

$$\langle \psi_{1s}(\vec{0}) \mid V' \mid \psi_{1s}(\vec{0}) \rangle = -5.1530.$$

Table A-I

Test Calculations of $\langle \Psi_\mu{}^s(\vec{A}) \mid \phi_\nu{}^s(\vec{B}) \rangle$

μ	α_1	A_x	A_y	A_z	ν	α_2	B_x	B_y	B_z	Overlap Integrals Calculated	Kotani
1s	3	1	2	3	1s	3	5	-6	4	+0.59265831E-10	+0.59265831E-10
2s	1	0	0	0	1s	2	0	0	3	+0.42882916E+00	+0.42882916E+00
$2p_x$	1	10	2	3	1s	2	1	2	3	-0.45919993E-02	-0.45919994E-02
2s	2	1	2	3	2s	2	5	-6	4	+0.14101826E-04	+0.14101827E-04
$2p_x$	2	1	2	3	2s	2	10	2	3	+0.12754352E-04	+0.12754353E-04
$2p_x$	2	1	2	3	$2p_x$	2	10	2	3	-0.11501375E-04	-0.11501376E-04

Table A-II

Test Calculations of $\langle \chi_\mu{}^s(\vec{A}) | -\frac{1}{2}\nabla^2 | \phi_\nu{}^s(\vec{B}) \rangle$

μ	α_1	A_x	A_y	A_z	ν	α_2	B_x	B_y	B_z	Kinetic Energy Integrals Calculated	Kotani
1s	3	1	2	3	1s	3	5	-6	4	-0.21158558E-09	-0.21158558E-09
2s	1	1	2	3	1s	2	-3	3	11	-0.12378458E-02	-0.12378458E-02
$2p_x$	1	10	2	3	1s	2	1	2	3	+0.11441893E-02	+0.11441893E-02
2s	2	1	2	3	2s	2	5	-6	4	-0.15057858E-04	-0.15057858E-04
$2p_x$	2	1	2	3	2s	2	10	2	3	-0.13200221E-04	-0.132002216E-04
$2p_x$	2	1	2	3	$2p_y$	2	-3	3	11	-0.60924406E-06	-0.60924410E-06

Table A-III

Test Calculations of $\langle \chi_\mu^{s}(\vec{A}) \mid V' = 1 \mid \phi_\nu^{s}(\vec{B}) \rangle$
(a_0 = 6.65 au)

μ	α_1	A_x	A_y	A_z	ν	α_2	B_x	B_y	B_z	Potential Energy Calculated	Overlap Kotani
1s	5	0	0	0	1s	5	0.05	0	0	2.4899E-02	2.4872E-02
2s	5	0	0	0	1s	5	0.05	0	0	7.5115E-03	7.5133E-03
2s	5	0	0	0	2s	5	0.05	0	0	3.0053E-03	3.0055E-03
$2p_x$	5	0	0	0	1s	5	0.05	0	0	6.2171E-04	6.2186E-04
$2p_x$	5	0	0	0	2s	5	0.05	0	0	1.2539E-04	1.2539E-04
$2p_y$	5	0	0	0	$2p_y$	5	0.05	0	0	9.9807E-04	9.9906E-04

TABLE A-IV

VALUES OF $\langle \phi_{2s}(0) | \phi_{1s}(\vec{B}) \rangle$, $\langle \phi_{2s}(0) | -\frac{1}{2}\nabla^2 | \phi_{1s}(\vec{B}) \rangle$, $\langle \phi_{2s}(0) | V | \phi_{1s}(\vec{B}) \rangle$ FOR $a_0 = 6.6500$ a.u

$\vec{B}/a_0$			MULTICENTER INTEGRALS		
$\frac{B_x}{a_0}$	$\frac{B_y}{a_0}$	$\frac{B_z}{a_0}$	OVERLAP	KINETIC ENERGY	POTENTIAL ENERGY
.0	.0	.0	.283891E-03	.682529E 00	-.649573E-00
.5	.5	.5	-.532376E-01	.560973E-03	.903769E-01
1.0	.0	.0	-.345968E-01	.122481E-02	.580141E-01
1.0	1.0	.0	-.813445E-02	.695059E-03	.133045E-01
1.5	.5	.5	-.329077E-02	.342795E-03	.533201E-02
1.0	1.0	1.0	-.249060E-02	.271117E-03	.402626E-02
2.0	.0	.0	-.890582E-03	.109662E-03	.142931E-02
1.5	1.5	.5	-.442089E-03	.578367E-04	.706009E-03
2.0	1.0	.0	-.353864E-03	.470664E-04	.564492E-03
2.0	1.0	1.0	-.151980E-03	.213313E-04	.241583E-03
2.5	.5	.5	-.839574E-04	.121556E-04	.133163E-03
1.5	1.5	1.5	-.839574E-04	.121556E-04	.133175E-03
2.0	2.0	.0	-.332272E-04	.500919E-05	.525531E-04
2.5	1.5	.5	-.196592E-04	.302198E-05	.310499E-04
2.0	2.0	1.0	-.165798E-04	.256364E-05	.261760E-04
3.0	.0	.0	-.165798E-04	.256364E-05	.261738E-04
3.0	1.0	.0	-.856256E-05	.135207E-05	.134968E-04
2.5	1.5	1.5	-.532005E-05	.851554E-06	.837797E-05
3.0	1.0	1.0	-.455514E-05	.732176E-06	.717087E-05
2.0	2.0	2.0	-.248687E-05	.405882E-06	.391076E-05

TABLE A-IV (CONT'D)

2.5	2.5	.5	-.160364E-05	.264398E-06	.251982E-05
3.5	.5	.5	-.160364E-05	.264398E-06	.251968E-05
3.0	2.0	.0	-.138916E-05	.229762E-06	.218226E-05
3.0	2.0	1.0	-.792007E-06	.132540E-06	.124311E-05
2.5	2.5	1.5	-.526012E-06	.887275E-07	.825153E-06
3.5	1.5	.5	-.526012E-06	.887275E-07	.825105E-06
4.0	.0	.0	-.271577E-06	.463559E-07	.425608E-06
3.5	1.5	1.5	-.184781E-06	.317435E-07	.289464E-06
3.0	2.0	2.0	-.162815E-06	.280270E-07	.255024E-06
4.0	1.0	.0	-.162815E-06	.280270E-07	.255003E-06
3.0	3.0	.0	-.989800E-07	.171697E-07	.154943E-06
4.0	1.0	1.0	-.989800E-07	.171697E-07	.154938E-06
2.5	2.5	2.5	-.687256E-07	.119852E-07	.107546E-06
3.5	2.5	.5	-.687256E-07	.119852E-07	.107540E-06
3.0	3.0	1.0	-.609500E-07	.106473E-07	.953636E-07
4.0	2.0	.0	-.379802E-07	.667767E-08	.593945E-07
3.5	2.5	1.5	-.268322E-07	.473894E-08	.419490E-07
4.5	.5	.5	-.268322E-07	.473894E-08	.419459E-07
4.0	2.0	1.0	-.239293E-07	.423236E-08	.374057E-07
3.0	3.0	2.0	-.152324E-07	.270904E-08	.238027E-07
4.5	1.5	.5	-.109245E-07	.195044E-08	.170650E-07
4.0	2.0	2.0	-.634915E-08	.114041E-08	.991414E-08
3.5	2.5	2.5	-.461415E-08	.831587E-09	.720343E-08
3.5	3.5	.5	-.461415E-08	.831587E-09	.720319E-08

TABLE A-V

VALUES OF $\langle \phi_{2s}(0) | \phi_{2s}(\vec{B}) \rangle$, $\langle \phi_{2s}(0) | -\frac{1}{2}\nabla^2 | \phi_{2s}(\vec{B}) \rangle$, $\langle \phi_{2s}(0) | V | \phi_{2s}(\vec{B}) \rangle$ FOR $a_0 = 6.6500\ a.u.$

$\vec{B}/a_0$			MULTICENTER INTEGRALS		
B_x/a_0	B_y/a_0	B_z/a_0	OVERLAP	KINETIC ENERGY	POTENTIAL ENERGY
.0	.0	.0	.100057E 01	.204844E 00	-.215818E-00
.5	.5	.5	.490032E-00	.158846E-01	-.424109E-01
1.0	.0	.0	.394464E-00	.884026E-02	-.393113E-01
1.0	1.0	.0	.172090E-00	-.160136E-02	-.222540E-01
1.5	.5	.5	.964646E-01	-.252156E-02	-.134778E-01
1.0	1.0	1.0	.801338E-01	-.247248E-02	-.116250E-01
2.0	.0	.0	.394201E-01	-.183532E-02	-.589115E-02
1.5	1.5	.5	.238541E-01	-.133349E-02	-.361709E-02
2.0	1.0	.0	.202767E-01	-.118965E-02	-.307545E-02
2.0	1.0	1.0	.108211E-01	-.740161E-03	-.167731E-02
2.5	.5	.5	.689717E-02	-.514303E-03	-.107741E-02
1.5	1.5	1.5	.689717E-02	-.514303E-03	-.108512E-02
2.0	2.0	.0	.336705E-02	-.280350E-03	-.531275E-03
2.5	1.5	.5	.222883E-02	-.195561E-03	-.353057E-03
2.0	2.0	1.0	.194765E-02	-.173599E-03	-.309451E-03
3.0	.0	.0	.194765E-02	-.173599E-03	-.309944E-03
3.0	1.0	.0	.114969E-02	-.108373E-03	-.183150E-03
2.5	1.5	1.5	.783559E-03	-.765651E-04	-.125475E-03
3.0	1.0	1.0	.691012E-03	-.682716E-04	-.110609E-03
2.0	2.0	2.0	.422102E-03	-.434137E-04	-.679891E-04

TABLE A-V (CONT'D)

2.5	2.5	.5	.294489E-03	-.311045E-04	-.473832E-04
3.5	.5	.5	.294489E-03	-.311045E-04	-.474004E-04
3.0	2.0	.0	.261640E-03	-.278647E-04	-.420926E-04
3.0	2.0	1.0	.164352E-03	-.180475E-04	-.265188E-04
2.5	2.5	1.5	.116903E-03	-.131050E-04	-.189111E-04
3.5	1.5	.5	.116903E-03	-.131050E-04	-.188816E-04
4.0	.0	.0	.672022E-04	-.776894E-05	-.108896E-04
3.5	1.5	1.5	.485893E-04	-.571131E-05	-.787765E-05
3.0	2.0	2.0	.436648E-04	-.515959E-05	-.708723E-05
4.0	1.0	.0	.436648E-04	-.515959E-05	-.707991E-05
3.0	3.0	.0	.286460E-04	-.345280E-05	-.465014E-05
4.0	1.0	1.0	.286460E-04	-.345280E-05	-.465076E-05
2.5	2.5	2.5	.210057E-04	-.256691E-05	-.341820E-05
3.5	2.5	.5	.210057E-04	-.256691E-05	-.341223E-05
3.0	3.0	1.0	.189625E-04	-.232741E-05	-.308249E-05
4.0	2.0	.0	.126582E-04	-.157967E-05	-.205851E-05
3.5	2.5	1.5	.939695E-05	-.118636E-05	-.153014E-05
4.5	.5	.5	.939695E-05	-.118636E-05	-.153008E-05
4.0	2.0	1.0	.851668E-05	-.107923E-05	-.138653E-05
3.0	3.0	2.0	.577274E-05	-.741961E-06	-.941355E-06
4.5	1.5	.5	.433227E-05	-.562391E-06	-.706214E-06
4.0	2.0	2.0	.270729E-05	-.356922E-06	-.441833E-06
3.5	2.5	2.5	.205154E-05	-.272824E-06	-.335097E-06
3.5	3.5	.5	.205154E-05	-.272824E-06	-.334863E-06

TABLE A-V (CONT'D)

4.5	1.5	1.5	.205154E-05	-.272824E-06	-.334880E-06
4.0	3.0	.0	.187179E-05	-.249617E-06	-.305524E-06
5.0	.0	.0	.187179E-05	-.249617E-06	-.305677E-06
4.0	3.0	1.0	.130183E-05	-.175484E-06	-.212636E-06
5.0	1.0	.0	.130183E-05	-.175484E-06	-.212656E-06
3.5	3.5	1.5	.995164E-06	-.135173E-06	-.162644E-06
4.5	2.5	.5	.995164E-06	-.135173E-06	-.162576E-06
3.0	3.0	3.0	.910551E-06	-.123985E-06	-.148920E-06
5.0	1.0	1.0	.910551E-06	-.123985E-06	-.148804E-06
4.5	2.5	1.5	.493354E-06	-.682815E-07	-.806842E-07
4.0	3.0	2.0	.452572E-06	-.627750E-07	-.740411E-07
5.0	2.0	.0	.452572E-06	-.627750E-07	-.740087E-07
5.0	2.0	1.0	.321453E-06	-.449683E-07	-.525902E-07
3.5	3.5	2.5	.249476E-06	-.351123E-07	-.408485E-07
5.5	.5	.5	.249476E-06	-.351123E-07	-.408341E-07
4.0	4.0	.0	.164434E-06	-.233669E-07	-.269196E-07
4.5	2.5	2.5	.128463E-06	-.183559E-07	-.210416E-07
4.5	3.5	.5	.128463E-06	-.183559E-07	-.210352E-07
5.5	1.5	.5	.128463E-06	-.183559E-07	-.210366E-07
4.0	4.0	1.0	.118378E-06	-.169450E-07	-.193871E-07
5.0	2.0	2.0	.118378E-06	-.169450E-07	-.193876E-07
4.0	3.0	3.0	.855751E-07	-.123347E-07	-.140245E-07
5.0	3.0	.0	.855751E-07	-.123347E-07	-.140164E-07
4.5	3.5	1.5	.672650E-07	-.974405E-08	-.110218E-07

TABLE A-VI

VALUES OF $\langle \phi_{2P_x}(0) \mid \phi_{1S}(\vec{B}) \rangle$, $\langle \phi_{2P_x}(0) \mid -\frac{1}{2}\nabla^2 \mid \phi_{1S}(\vec{B}) \rangle$, $\langle \phi_{2P_x}(0) \mid V \mid \phi_{1S}(\vec{B}) \rangle$ FOR $a_0 = 6.6500$ a.u.

$\vec{B}/a_0$			MULTICENTER INTEGRALS		
$\frac{B_x}{a_0}$	$\frac{B_y}{a_0}$	$\frac{B_z}{a_0}$	OVERLAP	KINETIC ENERGY	POTENTIAL ENERGY
.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
.5	.5	.5	.613473E-01	.320105E-02	-.107428E-00
1.0	.0	.0	.786523E-01	.214496E-02	-.136087E-00
1.0	1.0	.0	.195388E-01	-.398402E-03	-.330368E-01
1.5	.5	.5	.128098E-01	-.478069E-03	-.214828E-01
1.0	1.0	1.0	.664673E-02	-.275756E-03	-.111248E-01
2.0	.0	.0	.533828E-02	-.288346E-03	-.888106E-02
1.5	1.5	.5	.217076E-02	-.131684E-03	-.360012E-02
2.0	1.0	.0	.238567E-02	-.149190E-03	-.394895E-02
2.0	1.0	1.0	.115073E-02	-.791816E-04	-.189938E-02
2.5	.5	.5	.865502E-03	-.628021E-04	-.142615E-02
1.5	1.5	1.5	.519301E-03	-.376813E-04	-.855719E-03
2.0	2.0	.0	.314860E-03	-.244299E-04	-.517683E-03
2.5	1.5	.5	.252556E-03	-.202224E-04	-.414803E-03
2.0	2.0	1.0	.175009E-03	-.141456E-04	-.287349E-03
3.0	.0	.0	.262514E-03	-.212184E-04	-.431010E-03
3.0	1.0	.0	.150599E-03	-.125845E-04	-.246980E-03
2.5	1.5	1.5	.842227E-04	-.718902E-05	-.138024E-03
3.0	1.0	1.0	.887598E-04	-.762569E-05	-.145424E-03
2.0	2.0	2.0	.357011E-04	-.314034E-05	-.584459E-04

TABLE A-VII

VALUES OF $\langle \phi_{2P_y}(0) \mid \phi_{1S}(\vec{B}) \rangle$, $\langle \phi_{2P_y}(0) \mid -\frac{1}{2}\nabla^2 \mid \phi_{1S}(\vec{B}) \rangle$, $\langle \phi_{2P_y}(0) \mid V \mid \phi_{1S}(\vec{B}) \rangle$ FOR $a_o = 6.6500$ a.u.

$\vec{B}/a_o$			MULTICENTER INTEGRALS		
$\frac{B_x}{a_o}$	$\frac{B_y}{a_o}$	$\frac{B_z}{a_o}$	OVERLAP	KINETIC ENERGY	POTENTIAL ENERGY
.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
.5	.5	.5	.613473E-01	.320105E-02	-.107428E-00
1.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
1.0	1.0	.0	.195388E-01	-.398402E-03	-.330368E-01
1.5	.5	.5	.426993E-02	-.159356E-03	-.716072E-02
1.0	1.0	1.0	.664673E-02	-.275756E-03	-.111248E-01
2.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
1.5	1.5	.5	.217076E-02	-.131684E-03	-.360012E-02
2.0	1.0	.0	.119283E-02	-.745950E-04	-.197444E-02
2.0	1.0	1.0	.575367E-03	-.395908E-04	-.949678E-03
2.5	.5	.5	.173100E-03	-.125604E-04	-.285225E-03
1.5	1.5	1.5	.519301E-03	-.376813E-04	-.855719E-03
2.0	2.0	.0	.314860E-03	-.244299E-04	-.517683E-03
2.5	1.5	.5	.151533E-03	-.121334E-04	-.248879E-03
2.0	2.0	1.0	.175009E-03	-.141456E-04	-.287349E-03
3.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
3.0	1.0	.0	.501998E-04	-.419485E-05	-.823256E-04
2.5	1.5	1.5	.505336E-04	-.431341E-05	-.828142E-04
3.0	1.0	1.0	.295866E-04	-.254189E-05	-.484742E-04
2.0	2.0	2.0	.357011E-04	-.314034E-05	-.584459E-04

TABLE A-VIII

VALUES OF $\langle \phi_{2p_z}(0) | \phi_{1s}(\vec{B}) \rangle$, $\langle \phi_{2p_z}(0) | -\frac{1}{2}\nabla^2 | \phi_{1s}(\vec{B}) \rangle$, $\langle \phi_{2p_z}(0) | V | \phi_{1s}(\vec{B}) \rangle$ FOR $a_o = 6.6500$ a.u.

$\vec{B}/a_o$			MULTICENTER INTEGRALS		
$\frac{B_x}{a_o}$	$\frac{B_y}{a_o}$	$\frac{B_z}{a_o}$	OVERLAP	KINETIC ENERGY	POTENTIAL ENERGY
.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
.5	.5	.5	.613473E-01	.320105E-02	-.107428E-00
1.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
1.0	1.0	.0	.000000E-99	.000000E-99	.000000E-99
1.5	.5	.5	.426993E-02	-.159356E-03	-.716072E-02
1.0	1.0	1.0	.664673E-02	-.275756E-03	-.111248E-01
2.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
1.5	1.5	.5	.723588E-03	-.438948E-04	-.120001E-02
2.0	1.0	.0	.000000E-99	.000000E-99	.000000E-99
2.0	1.0	1.0	.575367E-03	-.395908E-04	-.949678E-03
2.5	.5	.5	.173100E-03	-.125604E-04	-.285225E-03
1.5	1.5	1.5	.519301E-03	-.376813E-04	-.855719E-03
2.0	2.0	.0	.000000E-99	.000000E-99	.000000E-99
2.5	1.5	.5	.505113E-04	-.404448E-05	-.829590E-04
2.0	2.0	1.0	.875048E-04	-.707281E-05	-.143672E-03
3.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
3.0	1.0	.0	.000000E-99	.000000E-99	.000000E-99
2.5	1.5	1.5	.505336E-04	-.431341E-05	-.828142E-04
3.0	1.0	1.0	.295866E-04	-.254189E-05	-.484742E-04
2.0	2.0	2.0	.357011E-04	-.314034E-05	-.584459E-04

TABLE A-IX

VALUES OF $\langle \phi_{2p_x}(0) | \phi_{2s}(\vec{B}) \rangle$, $\langle \phi_{2p_x}(0) | -\frac{1}{2}\nabla^2 | \phi_{2s}(\vec{B}) \rangle$, $\langle \phi_{2p_x}(0) | V | \phi_{2s}(\vec{B}) \rangle$ FOR $\zeta_0 = 6.6500$ a.u.

$\vec{B}/a_0$			MULTICENTER INTEGRALS		
B_x/a_0	B_y/a_0	B_z/a_0	OVERLAP	KINETIC ENERGY	POTENTIAL ENERGY
.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
.5	.5	.5	-.316028E-00	-.228719E-01	.284026E-01
1.0	.0	.0	-.504060E-00	-.301592E-01	.513389E-01
1.0	1.0	.0	-.218262E-00	-.538166E-02	.281643E-01
1.5	.5	.5	-.185975E-00	-.141911E-02	.256786E-01
1.0	1.0	1.0	-.103667E-00	-.311394E-03	.148505E-01
2.0	.0	.0	-.105383E-00	.126770E-02	.154394E-01
1.5	1.5	.5	-.492456E-01	.102062E-02	.731151E-02
2.0	1.0	.0	-.563940E-01	.131221E-02	.837431E-02
2.0	1.0	1.0	-.314339E-01	.100871E-02	.476081E-02
2.5	.5	.5	-.259166E-01	.974215E-03	.395272E-02
1.5	1.5	1.5	-.155499E-01	.584529E-03	.238725E-02
2.0	2.0	.0	-.107362E-01	.485548E-03	.165351E-02
2.5	1.5	.5	-.921007E-02	.452234E-03	.142447E-02
2.0	2.0	1.0	-.651696E-02	.327795E-03	.100950E-02
3.0	.0	.0	-.977545E-02	.491693E-03	.151394E-02
3.0	1.0	.0	-.605841E-02	.331266E-03	.941033E-03
2.5	1.5	1.5	-.356951E-02	.205591E-03	.557357E-03
3.0	1.0	1.0	-.382407E-02	.223741E-03	.596790E-03
2.0	2.0	2.0	-.163556E-02	.101231E-03	.256793E-03

TABLE A-IX (CONT'D)

2.5	2.5	.5	-.147977E-02	.949855E-04	.232216E-03
3.5	.5	.5	-.207168E-02	.132979E-03	.325137E-03
3.0	2.0	.0	-.159709E-02	.103672E-03	.250652E-03
3.0	2.0	1.0	-.105350E-02	.712451E-04	.165869E-03
2.5	2.5	1.5	-.647714E-03	.450101E-04	.102243E-03
3.5	1.5	.5	-.906800E-03	.630141E-04	.142917E-03
4.0	.0	.0	-.632998E-03	.457771E-04	.100071E-03
3.5	1.5	1.5	-.415234E-03	.306726E-04	.657207E-04
3.0	2.0	2.0	-.323717E-03	.240726E-04	.513006E-04
4.0	1.0	.0	-.431622E-03	.320968E-04	.683133E-04
3.0	3.0	.0	-.222809E-03	.169877E-04	.353150E-04
4.0	1.0	1.0	-.297079E-03	.226503E-04	.470901E-04
2.5	2.5	2.5	-.141114E-03	.109444E-04	.224237E-04
3.5	2.5	.5	-.197559E-03	.153222E-04	.313438E-04
3.0	3.0	1.0	-.154695E-03	.120629E-04	.245610E-04
4.0	2.0	.0	-.144369E-03	.114899E-04	.229351E-04
3.5	2.5	1.5	-.971510E-04	.784187E-05	.154586E-04
4.5	.5	.5	-.124908E-03	.100824E-04	.198817E-04
4.0	2.0	1.0	-.101817E-03	.825560E-05	.162089E-04
3.0	3.0	2.0	-.542394E-04	.447348E-05	.865112E-05
4.5	1.5	.5	-.632253E-04	.527695E-05	.100804E-04
4.0	2.0	2.0	-.372087E-04	.316288E-05	.594178E-05
3.5	2.5	2.5	-.255359E-04	.219282E-05	.408203E-05
3.5	3.5	.5	-.255359E-04	.219282E-05	.407828E-05

TABLE A-X

VALUES OF $\langle \phi_{2p_y}(0) \mid \phi_{2s}(\vec{B}) \rangle$, $\langle \phi_{2p_y}(0) \mid -\frac{1}{2}\nabla^2 \mid \phi_{2s}(\vec{B}) \rangle$, $\langle \phi_{2p_y}(0) \mid V \mid \phi_{2s}(\vec{B}) \rangle$ FOR $a_0 = 6.6500$ a.u.

$\vec{B}/a_0$			MULTICENTER INTEGRALS		
$\frac{B_x}{a_0}$	$\frac{B_y}{a_0}$	$\frac{B_z}{a_0}$	OVERLAP	KINETIC ENERGY	POTENTIAL ENERGY
.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
.5	.5	.5	-.316028E-00	-.228719E-01	.284026E-01
1.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
1.0	1.0	.0	-.218262E-00	-.538166E-02	.281643E-01
1.5	.5	.5	-.619918E-01	-.473037E-03	.858421E-02
1.0	1.0	1.0	-.103667E-00	-.311394E-03	.148505E-01
2.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
1.5	1.5	.5	-.492456E-01	.102062E-02	.731151E-02
2.0	1.0	.0	-.281970E-01	.656107E-03	.418760E-02
2.0	1.0	1.0	-.157169E-01	.504357E-03	.238191E-02
2.5	.5	.5	-.518332E-02	.194843E-03	.790581E-03
1.5	1.5	1.5	-.155499E-01	.584529E-03	.238725E-02
2.0	2.0	.0	-.107362E-01	.485548E-03	.165351E-02
2.5	1.5	.5	-.552604E-02	.271340E-03	.854704E-03
2.0	2.0	1.0	-.651696E-02	.327795E-03	.100950E-02
3.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
3.0	1.0	.0	-.201947E-02	.110422E-03	.313718E-03
2.5	1.5	1.5	-.214170E-01	.123355E-03	.334360E-03
3.0	1.0	1.0	-.127469E-02	.745805E-04	.198919E-03
2.0	2.0	2.0	-.163556E-02	.101231E-03	.256793E-03

TABLE A-X (CONT'D)

2.5	2.5	.5	-.147977E-02	.949855E-04	.232216E-03
3.5	.5	.5	-.295955E-03	.189971E-04	.464574E-04
3.0	2.0	.0	-.106472E-02	.691149E-04	.167094E-03
3.0	2.0	1.0	-.702335E-03	.474967E-04	.110569E-03
2.5	2.5	1.5	-.647714E-03	.450101E-04	.102243E-03
3.5	1.5	.5	-.388628E-03	.270060E-04	.612524E-04
4.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
3.5	1.5	1.5	-.177957E-03	.131454E-04	.281601E-04
3.0	2.0	2.0	-.215811E-03	.160484E-04	.341923E-04
4.0	1.0	.0	-.107905E-03	.802421E-05	.170819E-04
3.0	3.0	.0	-.222809E-03	.169877E-04	.353150E-04
4.0	1.0	1.0	-.742698E-04	.566258E-05	.117724E-04
2.5	2.5	2.5	-.141114E-03	.109444E-04	.224237E-04
3.5	2.5	.5	-.141114E-03	.109444E-04	.223871E-04
3.0	3.0	1.0	-.154695E-03	.120629E-04	.245610E-04
4.0	2.0	.0	-.721847E-04	.574497E-05	.114676E-04
3.5	2.5	1.5	-.693936E-04	.560134E-05	.110406E-04
4.5	.5	.5	-.138787E-04	.112026E-05	.220954E-05
4.0	2.0	1.0	-.509088E-04	.412780E-05	.810396E-05
3.0	3.0	2.0	-.542394E-04	.447348E-05	.865112E-05
4.5	1.5	.5	-.210751E-04	.175898E-05	.336039E-05
4.0	2.0	2.0	-.186043E-04	.158144E-05	.297024E-05
3.5	2.5	2.5	-.182399E-04	.156630E-05	.291521E-05
3.5	3.5	.5	-.255359E-04	.219282E-05	.407828E-05

TABLE A-XI

VALUES OF $\langle \phi_{2p_z}(0) \mid \phi_{2s}(\vec{B}) \rangle$, $\langle \phi_{2p_z}(0) \mid -\frac{1}{2}\nabla^2 \mid \phi_{2s}(\vec{B}) \rangle$, $\langle \phi_{2p_z}(0) \mid V \mid \phi_{2s}(\vec{B}) \rangle$ FOR $a_o = 6.6500$ a.u.

$\vec{B}/a_o$			MULTICENTER INTEGRALS		
$\frac{B_x}{a_o}$	$\frac{B_y}{a_o}$	$\frac{B_z}{a_o}$	OVERLAP	KINETIC ENERGY	POTENTIAL ENERGY
.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
.5	.5	.5	-.316028E-00	-.228719E-01	.284026E-01
1.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
1.0	1.0	.0	.000000E-99	.000000E-99	.000000E-99
1.5	.5	.5	-.619918E-01	-.473037E-03	.858421E-02
1.0	1.0	1.0	-.103667E-00	-.311394E-03	.148505E-01
2.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
1.5	1.5	.5	-.164152E-01	.340207E-03	.244351E-02
2.0	1.0	.0	.000000E-99	.000000E-99	.000000E-99
2.0	1.0	1.0	-.157169E-01	.504357E-03	.238191E-02
2.5	.5	.5	-.518332E-02	.194843E-03	.790581E-03
1.5	1.5	1.5	-.155499E-01	.584529E-03	.238725E-02
2.0	2.0	.0	.000000E-99	.000000E-99	.000000E-99
2.5	1.5	.5	-.184201E-02	.904468E-04	.284895E-03
2.0	2.0	1.0	-.325848E-02	.163897E-03	.504720E-03
3.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
3.0	1.0	.0	.000000E-99	.000000E-99	.000000E-99
2.5	1.5	1.5	-.214170E-02	.123355E-03	.334360E-03
3.0	1.0	1.0	-.127469E-02	.745805E-04	.198919E-03
2.0	2.0	2.0	-.163556E-02	.101231E-03	.256793E-03

TABLE A-XI (CONT'D)

2.5	2.5	.5	-.295955E-03	.189971E-04	.464222E-04
3.5	.5	.5	-.295955E-03	.189971E-04	.464574E-04
3.0	2.0	.0	.000000E-99	.000000E-99	.000000E-99
3.0	2.0	1.0	-.351167E-03	.237483E-04	.552666E-04
2.5	2.5	1.5	-.388628E-03	.270060E-04	.613249E-04
3.5	1.5	.5	-.129542E-03	.900202E-05	.204110E-04
4.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
3.5	1.5	1.5	-.177957E-03	.131454E-04	.281601E-04
3.0	2.0	2.0	-.215811E-03	.160484E-04	.341923E-04
4.0	1.0	.0	.000000E-99	.000000E-99	.000000E-99
3.0	3.0	.0	.000000E-99	.000000E-99	.000000E-99
4.0	1.0	1.0	-.742698E-04	.566258E-05	.117724E-04
2.5	2.5	2.5	-.141114E-03	.109444E-04	.224237E-04
3.5	2.5	.5	-.282228E-04	.218889E-05	.447539E-05
3.0	3.0	1.0	-.515650E-04	.402098E-05	.818304E-05
4.0	2.0	.0	.000000E-99	.000000E-99	.000000E-99
3.5	2.5	1.5	-.416361E-04	.336080E-05	.662249E-05
4.5	.5	.5	-.138787E-04	.112026E-05	.220954E-05
4.0	2.0	1.0	-.254544E-04	.206390E-05	.405090E-05
3.0	3.0	2.0	-.361596E-04	.298232E-05	.576588E-05
4.5	1.5	.5	.000000E-99	.000000E-99	.111988E-05
4.0	2.0	2.0	-.186043E-04	.158144E-05	.297024E-05
3.5	2.5	2.5	-.182399E-04	.156630E-05	.291521E-05
3.5	3.5	.5	-.364799E-05	.313260E-06	.582333E-06

TABLE A-XII

VALUES OF $\langle \phi_{2P_x}(0) \mid \phi_{2P_x}(\vec{B}) \rangle$, $\langle \phi_{2P_x}(0) \mid -\frac{1}{2}\nabla^2 \mid \phi_{2P_x}(\vec{B}) \rangle$, $\langle \phi_{2P_x}(0) \mid V \mid \phi_{2P_x}(\vec{B}) \rangle$ FOR $a_0 = 6.6500$ a.u.

$\vec{B}/a_0$			MULTICENTER INTEGRALS		
$\frac{B_x}{a_0}$	$\frac{B_y}{a_0}$	$\frac{B_z}{a_0}$	OVERLAP	KINETIC ENERGY	POTENTIAL ENERGY
.0	.0	.0	.999119E 00	.140902E-00	-.150679E-00
.5	.5	.5	.259914E-00	.551598E-02	-.412100E-01
1.0	.0	.0	-.253292E-00	-.437027E-01	.316082E-01
1.0	1.0	.0	-.726085E-01	-.935498E-02	.107175E-01
1.5	.5	.5	-.201628E-00	-.988397E-02	.316061E-01
1.0	1.0	1.0	-.234171E-01	-.275396E-02	.427457E-02
2.0	.0	.0	-.178034E-00	-.351770E-02	.288704E-01
1.5	1.5	.5	-.470372E-01	-.764870E-03	.764837E-02
2.0	1.0	.0	-.929835E-01	-.678417E-03	.149946E-01
2.0	1.0	1.0	-.509873E-01	.120004E-03	.829739E-02
2.5	.5	.5	-.586357E-01	.593051E-03	.956531E-02
1.5	1.5	1.5	-.136560E-01	.322575E-04	.227431E-02
2.0	2.0	.0	-.170848E-01	.283329E-03	.279501E-02
2.5	1.5	.5	-.208527E-01	.467816E-03	.340807E-02
2.0	2.0	1.0	-.103145E-01	.227496E-03	.169423E-02
3.0	.0	.0	-.284076E-01	.694515E-03	.465874E-02
3.0	1.0	.0	-.177251E-01	.515864E-03	.290296E-02
2.5	1.5	1.5	-.814377E-02	.256648E-03	.133689E-02
3.0	1.0	1.0	-.112752E-01	.374098E-03	.184869E-02
2.0	2.0	2.0	-.256907E-02	.888003E-04	.424377E-03

TABLE A-XII (CONT'D)

2.5	2.5	.5	-.341416E-02	.131730E-03	.560802E-03
3.5	.5	.5	-.756304E-02	.299417E-03	.124209E-02
3.0	2.0	.0	-.479190E-02	.191743E-03	.786279E-03
3.0	2.0	1.0	-.319058E-02	.136947E-03	.524079E-03
2.5	2.5	1.5	-.151415E-02	.670741E-04	.249291E-03
3.5	1.5	.5	-.338344E-02	.153125E-03	.555720E-03
4.0	.0	.0	-.282240E-02	.136856E-03	.464201E-03
3.5	1.5	1.5	-.158445E-02	.791737E-04	.260493E-03
3.0	2.0	2.0	-.100944E-02	.506627E-04	.166137E-03
4.0	1.0	.0	-.194796E-02	.987475E-04	.320295E-03
3.0	3.0	.0	-.701705E-03	.366515E-04	.115414E-03
4.0	1.0	1.0	-.135709E-02	.715538E-04	.223178E-03
2.5	2.5	2.5	-.339475E-03	.180192E-04	.559930E-04
3.5	2.5	.5	-.771060E-03	.416141E-04	.126801E-03
3.0	3.0	1.0	-.492047E-03	.266324E-04	.809771E-04
4.0	2.0	.0	-.675595E-03	.380781E-04	.111117E-03
3.5	2.5	1.5	-.387778E-03	.222682E-04	.638221E-04
4.5	.5	.5	-.678939E-03	.391834E-04	.111735E-03
4.0	2.0	1.0	-.482197E-03	.279667E-04	.793321E-04
3.0	3.0	2.0	-.177702E-03	.104971E-04	.292795E-04
4.5	1.5	.5	-.352235E-03	.213902E-04	.579682E-04
4.0	2.0	2.0	-.182539E-03	.113767E-04	.300510E-04
3.5	2.5	2.5	-.106500E-03	.672309E-05	.175446E-04
3.5	3.5	.5	-.106500E-03	.672309E-05	.175341E-04

TABLE A-XII (CONT'D)

4.5	1.5	1.5	-.187384E-03	.118793E-04	.308457E-04
4.0	3.0	.0	-.133660E-03	.850128E-05	.220012E-04
5.0	.0	.0	-.217921E-03	.138990E-04	.358837E-04
4.0	3.0	1.0	-.984100E-04	.637829E-05	.162024E-04
5.0	1.0	.0	-.160572E-03	.104351E-04	.264390E-04
3.5	3.5	1.5	-.578003E-04	.378710E-05	.952089E-05
4.5	2.5	.5	-.101936E-03	.670546E-05	.167814E-04
3.0	3.0	3.0	-.369804E-04	.242340E-05	.609769E-05
5.0	1.0	1.0	-.118933E-03	.786522E-05	.195834E-04
4.5	2.5	1.5	-.565746E-04	.384314E-05	.931641E-05
4.0	3.0	2.0	-.404831E-04	.275632E-05	.666867E-05
5.0	2.0	.0	-.662043E-04	.451857E-05	.109014E-04
5.0	2.0	1.0	-.497319E-04	.344330E-05	.818979E-05
3.5	3.5	2.5	-.180482E-04	.125675E-05	.297474E-05
5.5	.5	.5	-.493788E-04	.345620E-05	.813349E-05
4.0	4.0	.0	-.173399E-04	.122969E-05	.285614E-05
4.5	2.5	2.5	-.183697E-04	.131639E-05	.302624E-05
4.5	3.5	.5	-.183697E-04	.131639E-05	.302564E-05
5.5	1.5	.5	-.283980E-04	.203816E-05	.467760E-05

TABLE A-XIII

VALUES OF $\langle \phi_{2P_y}(0) \mid \phi_{2P_y}(\vec{B}) \rangle$, $\langle \phi_{2P_y}(0) \mid -\frac{1}{2}\nabla^2 \mid \phi_{2P_y}(\vec{B}) \rangle$, $\langle \phi_{2P_y}(0) \mid V \mid \phi_{2P_y}(\vec{B}) \rangle$ FOR $a_o = 6.6500$ a.u.

$\vec{B}/a_o$			MULTICENTER INTEGRALS		
$\frac{B_x}{a_o}$	$\frac{B_y}{a_o}$	$\frac{B_z}{a_o}$	OVERLAP	KINETIC ENERGY	POTENTIAL ENERGY
.0	.0	.0	.999119E 00	.140902E-00	-.150679E-00
.5	.5	.5	.259914E-00	.551598E-02	-.412100E-01
1.0	.0	.0	.376542E-00	.206394E-01	-.586476E-01
1.0	1.0	.0	-.726085E-01	-.935498E-02	.107175E-01
1.5	.5	.5	.714584E-01	.775459E-04	-.116510E-01
1.0	1.0	1.0	-.234171E-01	-.275396E-02	.427457E-02
2.0	.0	.0	.493187E-01	-.161372E-03	-.794948E-02
1.5	1.5	.5	-.470372E-01	-.764870E-03	.764837E-02
2.0	1.0	.0	-.201231E-02	-.433633E-03	.267744E-03
2.0	1.0	1.0	-.107940E-03	-.219266E-03	.308950E-04
2.5	.5	.5	.883379E-02	-.248139E-03	-.144743E-02
1.5	1.5	1.5	-.136560E-01	.322575E-04	.227431E-02
2.0	2.0	.0	-.170848E-01	.283329E-03	.279501E-02
2.5	1.5	.5	-.453711E-02	.671567E-04	.741424E-03
2.0	2.0	1.0	-.103145E-01	.227496E-03	.169423E-02
3.0	.0	.0	.415998E-02	-.146118E-03	-.680330E-03
3.0	1.0	.0	.444775E-03	-.366446E-04	-.745497E-04
2.5	1.5	1.5	-.165593E-02	.394818E-04	.274017E-03
3.0	1.0	1.0	.348532E-03	-.261290E-04	-.571997E-04
2.0	2.0	2.0	-.256907E-02	.888003E-04	.424377E-03

TABLE A-XIII (CONT'D)

2.5	2.5	.5	-.341416E-02	.131730E-03	.560802E-03
3.5	.5	.5	.734723E-03	-.359572E-04	-.120752E-03
3.0	2.0	.0	-.167115E-02	.632232E-04	.274297E-03
3.0	2.0	1.0	-.110209E-02	.449382E-04	.181284E-03
2.5	2.5	1.5	-.151415E-02	.670741E-04	.249291E-03
3.5	1.5	.5	-.267969E-03	.970688E-05	.439458E-04
4.0	.0	.0	.278209E-03	-.152169E-04	-.457193E-04
3.5	1.5	1.5	-.115700E-03	.470146E-05	.190876E-04
3.0	2.0	2.0	-.339074E-03	.163164E-04	.559613E-04
4.0	1.0	.0	.631492E-04	-.429127E-05	-.104186E-04
3.0	3.0	.0	-.701705E-03	.366515E-04	.115414E-03
4.0	1.0	1.0	.473162E-04	-.323683E-05	-.779268E-05
2.5	2.5	2.5	-.339475E-03	.180192E-04	.559930E-04
3.5	2.5	.5	-.339475E-03	.180192E-04	.558502E-04
3.0	3.0	1.0	-.492047E-03	.266324E-04	.809771E-04
4.0	2.0	.0	-.113715E-03	.612597E-05	.186994E-04
3.5	2.5	1.5	-.169407E-03	.958182E-05	.279077E-04
4.5	.5	.5	.489632E-04	-.310458E-05	-.805937E-05
4.0	2.0	1.0	-.802767E-04	.445764E-05	.132148E-04
3.0	3.0	2.0	-.177702E-03	.104971E-04	.292795E-04
4.5	1.5	.5	-.112318E-04	.556817E-06	.184554E-05
4.0	2.0	2.0	-.294194E-04	.176234E-05	.485163E-05
3.5	2.5	2.5	-.458377E-04	.285587E-05	.756041E-05
3.5	3.5	.5	-.106500E-03	.672309E-05	.175341E-04

TABLE A-XIII (CONT'D)

4.5	1.5	1.5	-.539590E-05	.277729E-06	.889300E-06
4.0	3.0	.0	-.681243E-04	.430302E-05	.112160E-04
5.0	.0	.0	.161362E-04	-.109474E-05	-.265637E-05
4.0	3.0	1.0	-.500611E-04	.322292E-05	.824494E-05
5.0	1.0	.0	.519479E-05	-.383204E-06	-.856036E-06
3.5	3.5	1.5	-.578003E-04	.378710E-05	.952089E-05
4.5	2.5	.5	-.246984E-04	.159832E-05	.406675E-05
3.0	3.0	3.0	-.369804E-04	.242340E-05	.609769E-05
5.0	1.0	1.0	.399592E-05	-.297497E-06	-.658419E-06
4.5	2.5	1.5	-.135801E-04	.908295E-06	.223767E-05
4.0	3.0	2.0	-.204777E-04	.138567E-05	.337509E-05
5.0	2.0	.0	-.618818E-05	.406650E-06	.101869E-05
5.0	2.0	1.0	-.459668E-05	.306632E-06	.757088E-06
3.5	3.5	2.5	-.180482E-04	.125675E-05	.297474E-05
5.5	.5	.5	.283885E-05	-.209542E-06	-.467629E-06
4.0	4.0	.0	-.173399E-04	.122969E-05	.285614E-05
4.5	2.5	2.5	-.432998E-05	.305915E-06	.714022E-06
4.5	3.5	.5	-.103470E-04	.738979E-06	.170449E-05
5.5	1.5	.5	-.318632E-06	.172072E-07	.523924E-07

TABLE A-XIV

VALUES OF $\langle \phi_{2p_z}(0) | \phi_{2p_z}(\vec{B}) \rangle$, $\langle \phi_{2p_z}(0) | -\frac{1}{2}\nabla^2 | \phi_{2p_z}(\vec{B}) \rangle$, $\langle \phi_{2p_z}(0) | V | \phi_{2p_z}(\vec{B}) \rangle$ FOR $a_0 = 6.6500\ a.u.$

$\vec{B}/a_0$			MULTICENTER INTEGRALS		
$\frac{B_x}{a_0}$	$\frac{B_y}{a_0}$	$\frac{B_z}{a_0}$	OVERLAP	KINETIC ENERGY	POTENTIAL ENERGY
.0	.0	.0	.999119E 00	.140902E-00	-.150679E-00
.5	.5	.5	.259914E-00	.551598E-02	-.412100E-01
1.0	.0	.0	.376542E-00	.206394E-01	-.586476E-01
1.0	1.0	.0	.175219E-00	.457466E-02	-.294486E-01
1.5	.5	.5	.714584E-01	.775459E-04	-.116510E-01
1.0	1.0	1.0	-.234171E-01	-.275396E-02	.427457E-02
2.0	.0	.0	.493187E-01	-.161372E-03	-.794948E-02
1.5	1.5	.5	.235775E-01	-.383107E-03	-.390398E-02
2.0	1.0	.0	.283114E-01	-.352038E-03	-.467645E-02
2.0	1.0	1.0	-.107940E-03	-.219266E-03	.308950E-04
2.5	.5	.5	.883379E-02	-.248139E-03	-.144743E-02
1.5	1.5	1.5	-.136560E-01	.322575E-04	.227431E-02
2.0	2.0	.0	.648730E-02	-.199654E-03	-.107413E-02
2.5	1.5	.5	.362072E-02	-.133172E-03	-.597486E-03
2.0	2.0	1.0	.541361E-03	-.527143E-04	-.874370E-04
3.0	.0	.0	.415998E-02	-.146118E-03	-.680330E-03
3.0	1.0	.0	.271601E-02	-.105708E-03	-.447135E-03
2.5	1.5	1.5	-.165593E-02	.394818E-04	.274017E-03
3.0	1.0	1.0	.348532E-03	-.261290E-04	-.571997E-04
2.0	2.0	2.0	-.256907E-02	.888003E-04	.424377E-03

TABLE A-XIV (CONT'D)

2.5	2.5	.5	.734723E-03	-.359572E-04	-.121347E-03
3.5	.5	.5	.734723E-03	-.359572E-04	-.120752E-03
3.0	2.0	.0	.825444E-03	-.395929E-04	-.136293E-03
3.0	2.0	1.0	.151001E-03	-.102673E-04	-.248278E-04
2.5	2.5	1.5	-.267969E-03	.970688E-05	.443867E-04
3.5	1.5	.5	.355124E-03	-.189767E-04	-.585290E-04
4.0	.0	.0	.278209E-03	-.152169E-04	-.457193E-04
3.5	1.5	1.5	-.115700E-03	.470146E-05	.190876E-04
3.0	2.0	2.0	-.339074E-03	.163164E-04	.559613E-04
4.0	1.0	.0	.197223E-03	-.111605E-04	-.324709E-04
3.0	3.0	.0	.140943E-03	-.822288E-05	-.232715E-04
4.0	1.0	1.0	.473162E-04	-.323683E-05	-.779268E-05
2.5	2.5	2.5	-.339475E-03	.180192E-04	.559930E-04
3.5	2.5	.5	.921095E-04	-.557569E-05	-.151990E-04
3.0	3.0	1.0	.355331E-04	-.245068E-05	-.585518E-05
4.0	2.0	.0	.735782E-04	-.452475E-05	-.121343E-04
3.5	2.5	1.5	-.238270E-04	.112421E-05	.393937E-05
4.5	.5	.5	.489632E-04	-.310458E-05	-.805937E-05
4.0	2.0	1.0	.202033E-04	-.141962E-05	-.332884E-05
3.0	3.0	2.0	-.570745E-04	.325777E-05	.942383E-05
4.5	1.5	.5	.266574E-04	-.175800E-05	-.439277E-05
4.0	2.0	2.0	-.294194E-04	.176234E-05	.485163E-05
3.5	2.5	2.5	-.458377E-04	.285587E-05	.756041E-05
3.5	3.5	.5	.148250E-04	-.101134E-05	-.244630E-05

TABLE A-XIV (CONT'D)

4.5	1.5	1.5	-.539590E-05	.277729E-06	.889300E-06
4.0	3.0	.0	.161362E-04	-.109474E-05	-.266254E-05
5.0	.0	.0	.161362E-04	-.109474E-05	-.265637E-05
4.0	3.0	1.0	.519479E-05	-.383204E-06	-.856509E-06
5.0	1.0	.0	.121017E-04	-.833971E-06	-.199340E-05
3.5	3.5	1.5	-.263059E-05	.139141E-06	.434960E-06
4.5	2.5	.5	.840335E-05	-.590449E-06	-.138588E-05
3.0	3.0	3.0	-.369804E-04	.242340E-05	.609769E-05
5.0	1.0	1.0	.399592E-05	-.297497E-06	-.658419E-06
4.5	2.5	1.5	-.129597E-05	.697682E-07	.214017E-06
4.0	3.0	2.0	-.618818E-05	.406650E-06	.102123E-05
5.0	2.0	.0	.524346E-05	-.376573E-06	-.864430E-06
5.0	2.0	1.0	.185121E-05	-.141463E-06	-.305132E-06
3.5	3.5	2.5	-.760468E-05	.523607E-06	.125462E-05
5.5	.5	.5	.283885E-05	-.209542E-06	-.467629E-06
4.0	4.0	.0	.235504E-05	-.175086E-06	-.388561E-06
4.5	2.5	2.5	-.432998E-05	.305915E-06	.714022E-06
4.5	3.5	.5	.168704E-05	-.127147E-06	-.278300E-06
5.5	1.5	.5	.168704E-05	-.127147E-06	-.278033E-06

TABLE A-XV

VALUES OF $\langle \phi_{2P_y}(0) | \phi_{2P_x}(\vec{B}) \rangle$, $\langle \phi_{2P_y}(0) | -\frac{1}{2}\nabla^2 | \phi_{2P_x}(\vec{B}) \rangle$, $\langle \phi_{2P_y}(0) | V | \phi_{2P_x}(\vec{B}) \rangle$ FOR $a_0 = 6.6500\ a.u.$

$\vec{B}/a_0$			MULTICENTER INTEGRALS		
B_x/a_0	B_y/a_0	B_z/a_0	OVERLAP	KINETIC ENERGY	POTENTIAL ENERGY
.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
.5	.5	.5	-.207007E 00	-.252474E-01	.280842E-01
1.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
1.0	1.0	.0	-.247828E 00	-.139296E-01	.381772E-01
1.5	.5	.5	-.102407E 00	-.373556E-02	.164728E-01
1.0	1.0	1.0	-.113439E-00	-.354858E-02	.183950E-01
2.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
1.5	1.5	.5	-.794417E-01	-.429484E-03	.128629E-01
2.0	1.0	.0	-.606474E-01	-.163189E-03	.983054E-02
2.0	1.0	1.0	-.339196E-01	.226180E-03	.555173E-02
2.5	.5	.5	-.140561E-01	.175248E-03	.229871E-02
1.5	1.5	1.5	-.253010E-01	.315446E-03	.415487E-02
2.0	2.0	.0	-.235721E-01	.482983E-03	.385178E-02
2.5	1.5	.5	-.152959E-01	.375618E-03	.250383E-02
2.0	2.0	1.0	-.144744E-01	.373614E-03	.237226E-02
3.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
3.0	1.0	.0	-.681372E-02	.207190E-03	.111667E-02
2.5	1.5	1.5	-.608235E-02	.203593E-03	.999931E-03
3.0	1.0	1.0	-.435890E-02	.150085E-03	.716055E-03
2.0	2.0	2.0	-.378087E-02	.143657E-03	.622334E-03

TABLE A-XV (CONT'D)

2.5	2.5	.5	-.432175E-02	.174674E-03	.709506E-03
3.5	.5	.5	-.121009E-02	.489088E-04	.198803E-03
3.0	2.0	.0	-.374489E-02	.154224E-03	.614802E-03
3.0	2.0	1.0	-.250618E-02	.110411E-03	.411887E-03
2.5	2.5	1.5	-.194716E-02	.896363E-04	.320264E-03
3.5	1.5	.5	-.163562E-02	.752945E-04	.268797E-03
4.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
3.5	1.5	1.5	-.771097E-03	.390979E-04	.126906E-03
3.0	2.0	2.0	-.804446E-03	.412155E-04	.132454E-03
4.0	1.0	.0	-.536297E-03	.274770E-04	.881883E-04
3.0	3.0	.0	-.842649E-03	.448744E-04	.138569E-03
4.0	1.0	1.0	-.374510E-03	.199441E-04	.616270E-04
2.5	2.5	2.5	-.449567E-03	.245780E-04	.740605E-04
3.5	2.5	.5	-.629394E-03	.344092E-04	.103526E-03
3.0	3.0	1.0	-.593528E-03	.327185E-04	.976495E-04
4.0	2.0	.0	-.374586E-03	.213014E-04	.616266E-04
3.5	2.5	1.5	-.318457E-03	.185010E-04	.524242E-04
4.5	.5	.5	-.818890E-04	.475740E-05	.134774E-04
4.0	2.0	1.0	-.267946E-03	.156727E-04	.441008E-04
3.0	3.0	2.0	-.217130E-03	.130308E-04	.357587E-04
4.5	1.5	.5	-.127876E-03	.781253E-05	.210489E-04
4.0	2.0	2.0	-.102079E-03	.640957E-05	.168146E-04
3.5	2.5	2.5	-.884666E-04	.563969E-05	.145759E-04
3.5	3.5	.5	-.123853E-03	.789557E-05	.203889E-04

TABLE A-XV (CONT'D)

4.5	1.5	1.5	-.682456E-04	.435062E-05	.112397E-04
4.0	3.0	.0	-.112347E-03	.719702E-05	.184947E-04
5.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
4.0	3.0	1.0	-.828838E-04	.540919E-05	.136475E-04
5.0	1.0	.0	-.345349E-04	.225383E-05	.568634E-05
3.5	3.5	1.5	-.675829E-04	.446874E-05	.111303E-04
4.5	2.5	.5	-.620659E-04	.410395E-05	.102195E-04
3.0	3.0	3.0	-.460984E-04	.306101E-05	.759713E-05
5.0	1.0	1.0	-.256102E-04	.170056E-05	.421789E-05
4.5	2.5	1.5	-.345491E-04	.235835E-05	.569085E-05
4.0	3.0	2.0	-.342949E-04	.234967E-05	.564984E-05
5.0	2.0	.0	-.285791E-04	.195805E-05	.470650E-05
5.0	2.0	1.0	-.214929E-04	.149365E-05	.354016E-05
3.5	3.5	2.5	-.213222E-04	.149684E-05	.351347E-05
5.5	.5	.5	-.478661E-05	.336027E-06	.788438E-06
4.0	4.0	.0	-.196949E-04	.140477E-05	.324388E-05
4.5	2.5	2.5	-.112819E-04	.811993E-06	.185917E-05
4.5	3.5	.5	-.157946E-04	.113679E-05	.260164E-05
5.5	1.5	.5	-.827340E-05	.595461E-06	.136285E-05
4.0	4.0	1.0	-.149929E-04	.108224E-05	.246973E-05
5.0	2.0	2.0	-.937059E-05	.676404E-06	.154403E-05
4.0	3.0	3.0	-.859195E-05	.627256E-06	.141609E-05
5.0	3.0	.0	-.107399E-04	.784070E-06	.176913E-05
4.5	3.5	1.5	-.923776E-05	.679891E-06	.152195E-05

TABLE A-XVI

VALUES OF $\langle \phi_{2p_z}(0) | \phi_{2p_x}(\vec{B}) \rangle$, $\langle \phi_{2p_z}(0) | -\frac{1}{2}\nabla^2 | \phi_{2p_x}(\vec{B}) \rangle$, $\langle \phi_{2p_z}(0) | V | \phi_{2p_x}(\vec{B}) \rangle$ FOR $a_o = 6.6500$ a.u.

$\vec{B}/a_o$			MULTICENTER INTEGRALS		
$\frac{B_x}{a_o}$	$\frac{B_y}{a_o}$	$\frac{B_z}{a_o}$	OVERLAP	KINETIC ENERGY	POTENTIAL ENERGY
.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
.5	.5	.5	-.207007E 00	-.252474E-01	.280842E-01
1.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
1.0	1.0	.0	.000000E-99	.000000E-99	.000000E-99
1.5	.5	.5	-.102407E-00	-.373556E-02	.164728E-01
1.0	1.0	1.0	-.113439E-00	-.354858E-02	.183950E-01
2.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
1.5	1.5	.5	-.264805E-01	-.143161E-03	.433808E-02
2.0	1.0	.0	.000000E-99	.000000E-99	.000000E-99
2.0	1.0	1.0	-.339196E-01	.226180E-03	.555173E-02
2.5	.5	.5	-.140561E-01	.175248E-03	.229871E-02
1.5	1.5	1.5	-.253010E-01	.315446E-03	.415487E-02
2.0	2.0	.0	.000000E-99	.000000E-99	.000000E-99
2.5	1.5	.5	-.509864E-02	.125206E-03	.837774E-03
2.0	2.0	1.0	-.723724E-02	.186807E-03	.119043E-02
3.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
3.0	1.0	.0	.000000E-99	.000000E-99	.000000E-99
2.5	1.5	1.5	-.608235E-02	.203593E-03	.999931E-03
3.0	1.0	1.0	-.435890E-02	.150085E-03	.716055E-03
2.0	2.0	2.0	-.378087E-02	.143657E-03	.622334E-03

TABLE A-XVI (CONT'D)

2.5	2.5	.5	-.864351E-03	.349348E-04	.142320E-03
3.5	.5	.5	-.121009E-02	.489088E-04	.198803E-03
3.0	2.0	.0	.000000E-99	.000000E-99	.000000E-99
3.0	2.0	1.0	-.125309E-02	.552056E-04	.206289E-03
2.5	2.5	1.5	-.116830E-02	.537818E-04	.192416E-03
3.5	1.5	.5	-.545207E-03	.250981E-04	.897176E-04
4.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
3.5	1.5	1.5	-.771097E-03	.390979E-04	.126906E-03
3.0	2.0	2.0	-.804446E-03	.412155E-04	.132454E-03
4.0	1.0	.0	.000000E-99	.000000E-99	.000000E-99
3.0	3.0	.0	.000000E-99	.000000E-99	.000000E-99
4.0	1.0	1.0	-.374510E-03	.199441E-04	.616270E-04
2.5	2.5	2.5	-.449567E-03	.245780E-04	.740605E-04
3.5	2.5	.5	-.125878E-03	.688185E-05	.207370E-04
3.0	3.0	1.0	-.197842E-03	.109061E-04	.325971E-04
4.0	2.0	.0	.000000E-99	.000000E-99	.000000E-99
3.5	2.5	1.5	-.191074E-03	.111006E-04	.314793E-04
4.5	.5	.5	-.818890E-04	.475740E-05	.134774E-04
4.0	2.0	1.0	-.133973E-03	.783636E-05	.220665E-04
3.0	3.0	2.0	-.144753E-03	.868724E-05	.238531E-04
4.5	1.5	.5	-.426254E-04	.260417E-05	.701982E-05
4.0	2.0	2.0	-.102079E-03	.640957E-05	.168146E-04
3.5	2.5	2.5	-.884666E-04	.563969E-05	.145759E-04
3.5	3.5	.5	-.176933E-04	.112793E-05	.291600E-05

TABLE A-XVI (CONT'D)

4.5	1.5	1.5	-.682456E-04	.435062E-05	.112397E-04
4.0	3.0	.0	.000000E-99	.000000E-99	.000000E-99
5.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
4.0	3.0	1.0	-.276279E-04	.180306E-05	.455316E-05
5.0	1.0	.0	.000000E-99	.000000E-99	.000000E-99
3.5	3.5	1.5	-.289641E-04	.191517E-05	.477377E-05
4.5	2.5	.5	-.124131E-04	.820790E-06	.204545E-05
3.0	3.0	3.0	-.460984E-04	.306101E-05	.759713E-05
5.0	1.0	1.0	-.256102E-04	.170056E-05	.421789E-05
4.5	2.5	1.5	-.207295E-04	.141501E-05	.341590E-05
4.0	3.0	2.0	-.228633E-04	.156644E-05	.376807E-05
5.0	2.0	.0	.000000E-99	.000000E-99	.000000E-99
5.0	2.0	1.0	-.107464E-04	.746826E-06	.177066E-05
3.5	3.5	2.5	-.152301E-04	.106917E-05	.251036E-05
5.5	.5	.5	-.478661E-05	.336027E-06	.788438E-06
4.0	4.0	.0	.000000E-99	.000000E-99	.000000E-99
4.5	2.5	2.5	-.112819E-04	.811993E-06	.185917E-05
4.5	3.5	.5	-.225638E-05	.162398E-06	.371931E-06
5.5	1.5	.5	-.275780E-05	.198487E-06	.454380E-06
4.0	4.0	1.0	-.374823E-05	.270561E-06	.617861E-06
5.0	2.0	2.0	-.937059E-05	.676404E-06	.154403E-05
4.0	3.0	3.0	-.859195E-05	.627256E-06	.141609E-05
5.0	3.0	.0	.000000E-99	.000000E-99	.000000E-99
4.5	3.5	1.5	-.395904E-05	.291382E-06	.652598E-06

TABLE A-XVII

VALUES OF $\langle \phi_{2p_z}(0) | \phi_{2p_y}(\vec{B}) \rangle$, $\langle \phi_{2p_z}(0) | -\frac{1}{2}\nabla^2 | \phi_{2p_y}(\vec{B}) \rangle$, $\langle \phi_{2p_z}(0) | V | \phi_{2p_y}(\vec{B}) \rangle$ FOR $a_o = 6.6500\ a.u.$

$\vec{B}/a_o$			MULTICENTER INTEGRALS		
$\frac{B_x}{a_o}$	$\frac{B_y}{a_o}$	$\frac{B_z}{a_o}$	OVERLAP	KINETIC ENERGY	POTENTIAL ENERGY
.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
.5	.5	.5	-.207007E 00	-.252474E-01	.280842E-01
1.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
1.0	1.0	.0	.000000E-99	.000000E-99	.000000E-99
1.5	.5	.5	-.341359E-01	-.124518E-02	.509492E-02
1.0	1.0	1.0	-.113439E-00	-.354858E-02	.183950E-01
2.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
1.5	1.5	.5	-.264805E-01	-.143161E-03	.433808E-02
2.0	1.0	.0	.000000E-99	.000000E-99	.000000E-99
2.0	1.0	1.0	-.169598E-01	.113090E-03	.275798E-02
2.5	.5	.5	-.281123E-02	.350496E-04	.446508E-03
1.5	1.5	1.5	-.253010E-01	.315446E-03	.415487E-02
2.0	2.0	.0	.000000E-99	.000000E-99	.000000E-99
2.5	1.5	.5	-.305918E-02	.751236E-04	.501276E-03
2.0	2.0	1.0	-.723724E-02	.186807E-03	.119043E-02
3.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
3.0	1.0	.0	.000000E-99	.000000E-99	.000000E-99
2.5	1.5	1.5	-.364941E-02	.122156E-03	.599719E-03
3.0	1.0	1.0	-.145296E-02	.500284E-04	.237648E-03
2.0	2.0	2.0	-.378087E-02	.143657E-03	.622334E-03

TABLE A-XVII (CONT'D)

2.5	2.5	.5	-.864351E-03	.349348E-04	.142320E-03
3.5	.5	.5	-.172870E-03	.698697E-05	.281228E-04
3.0	2.0	.0	.000000E-99	.000000E-99	.000000E-99
3.0	2.0	1.0	-.835396E-03	.368037E-04	.137442E-03
2.5	2.5	1.5	-.116830E-02	.537818E-04	.192416E-03
3.5	1.5	.5	-.233660E-03	.107563E-04	.383626E-04
4.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
3.5	1.5	1.5	-.330470E-03	.167562E-04	.543522E-04
3.0	2.0	2.0	-.536297E-03	.274770E-04	.883228E-04
4.0	1.0	.0	.000000E-99	.000000E-99	.000000E-99
3.0	3.0	.0	.000000E-99	.000000E-99	.000000E-99
4.0	1.0	1.0	-.936276E-04	.498604E-05	.153719E-04
2.5	2.5	2.5	-.449567E-03	.245780E-04	.740605E-04
3.5	2.5	.5	-.899135E-04	.491561E-05	.148070E-04
3.0	3.0	1.0	-.197842E-03	.109061E-04	.325971E-04
4.0	2.0	.0	.000000E-99	.000000E-99	.000000E-99
3.5	2.5	1.5	-.136481E-03	.792900E-05	.224832E-04
4.5	.5	.5	-.909878E-05	.528600E-06	.149228E-05
4.0	2.0	1.0	-.669867E-04	.391818E-05	.110260E-04
3.0	3.0	2.0	-.144753E-03	.868724E-05	.238531E-04
4.5	1.5	.5	-.142084E-04	.868059E-06	.233671E-05
4.0	2.0	2.0	-.510399E-04	.320478E-05	.840748E-05
3.5	2.5	2.5	-.631904E-04	.402835E-05	.104135E-04
3.5	3.5	.5	-.176933E-04	.112793E-05	.291600E-05

TABLE A-XVII (CONT'D)

4.5	1.5	1.5	-.227485E-04	.145020E-05	.374454E-05
4.0	3.0	.0	.000000E-99	.000000E-99	.000000E-99
5.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
4.0	3.0	1.0	-.207209E-04	.135229E-05	.341450E-05
5.0	1.0	.0	.000000E-99	.000000E-99	.000000E-99
3.5	3.5	1.5	-.289641E-04	.191517E-05	.477377E-05
4.5	2.5	.5	-.689621E-05	.455994E-06	.113592E-05
3.0	3.0	3.0	-.460984E-04	.306101E-05	.759713E-05
5.0	1.0	1.0	-.512205E-05	.340113E-06	.842607E-06
4.5	2.5	1.5	-.115163E-04	.786119E-06	.189743E-05
4.0	3.0	2.0	-.171474E-04	.117483E-05	.282613E-05
5.0	2.0	.0	.000000E-99	.000000E-99	.000000E-99
5.0	2.0	1.0	-.429859E-05	.298730E-06	.707920E-06
3.5	3.5	2.5	-.152301E-04	.106917E-05	.251036E-05
5.5	.5	.5	-.435147E-06	.305479E-07	.715748E-07
4.0	4.0	.0	.000000E-99	.000000E-99	.000000E-99
4.5	2.5	2.5	-.626773E-05	.451107E-06	.103300E-05
4.5	3.5	.5	-.175496E-05	.126310E-06	.289259E-06
5.5	1.5	.5	-.752128E-06	.541328E-07	.123825E-06
4.0	4.0	1.0	-.374823E-05	.270561E-06	.617861E-06
5.0	2.0	2.0	-.374823E-05	.270561E-06	.617564E-06
4.0	3.0	3.0	-.644396E-05	.470442E-06	.106221E-05
5.0	3.0	.0	.000000E-99	.000000E-99	.000000E-99
4.5	3.5	1.5	-.307925E-05	.226630E-06	.507565E-06

TABLE A-XVIII

VALUES OF $\langle \phi_{2s}(0) | \phi_{1s}(\vec{B}) \rangle$, $\langle \phi_{2s}(0) | -\frac{1}{2}\nabla^2 | \phi_{1s}(\vec{B}) \rangle$, $\langle \phi_{2s}(0) | V | \phi_{1s}(\vec{B}) \rangle$ FOR $a_0 = 6.5183$

$\vec{B}/a_0$			MULTICENTER INTEGRALS		
$\frac{B_x}{a_0}$	$\frac{B_y}{a_0}$	$\frac{B_z}{a_0}$	OVERLAP	KINETIC ENERGY	POTENTIAL ENERGY
.0	.0	.0	.283891E-03	.682529E 00	-.64[illegible]
.5	.5	.5	-.561511E-01	.385883E-03	.95[illegible]
1.0	.0	.0	-.369279E-01	.118525E-02	.62[illegible]
1.0	1.0	.0	-.900667E-02	.746772E-03	.14[illegible]
1.5	.5	.5	-.372288E-02	.379560E-03	.6[illegible]
1.0	1.0	1.0	-.283599E-02	.302665E-03	.45[illegible]
2.0	.0	.0	-.103826E-02	.125897E-03	.16[illegible]
1.5	1.5	.5	-.523589E-03	.675896E-04	.83[illegible]
2.0	1.0	.0	-.421188E-03	.553064E-04	.67[illegible]
2.0	1.0	1.0	-.184315E-03	.255822E-04	.29[illegible]
2.5	.5	.5	-.103155E-03	.147829E-04	.16[illegible]
1.5	1.5	1.5	-.103155E-03	.147829E-04	.16[illegible]
2.0	2.0	.0	-.416579E-04	.622336E-05	.65[illegible]
2.5	1.5	.5	-.249289E-04	.379943E-05	.39[illegible]
2.0	2.0	1.0	-.211015E-04	.323558E-05	.33[illegible]
3.0	.0	.0	-.211015E-04	.323558E-05	.33[illegible]
3.0	1.0	.0	-.110537E-04	.173188E-05	.17[illegible]
2.5	1.5	1.5	-.693826E-05	.110234E-05	.10[illegible]
3.0	1.0	1.0	-.596045E-05	.951070E-06	.93[illegible]
2.0	2.0	2.0	-.329639E-05	.534296E-06	.51[illegible]

TABLE A-XVII (CONT'D)

4.5	1.5	1.5	-.227485E-04	.145020E-05	.374454E-05
4.0	3.0	.0	.000000E-99	.000000E-99	.000000E-99
5.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
4.0	3.0	1.0	-.207209E-04	.135229E-05	.341450E-05
5.0	1.0	.0	.000000E-99	.000000E-99	.000000E-99
3.5	3.5	1.5	-.289641E-04	.191517E-05	.477377E-05
4.5	2.5	.5	-.689621E-05	.455994E-06	.113592E-05
3.0	3.0	3.0	-.460984E-04	.306101E-05	.759713E-05
5.0	1.0	1.0	-.512205E-05	.340113E-06	.842607E-06
4.5	2.5	1.5	-.115163E-04	.786119E-06	.189743E-05
4.0	3.0	2.0	-.171474E-04	.117483E-05	.282613E-05
5.0	2.0	.0	.000000E-99	.000000E-99	.000000E-99
5.0	2.0	1.0	-.429859E-05	.298730E-06	.707920E-06
3.5	3.5	2.5	-.152301E-04	.106917E-05	.251036E-05
5.5	.5	.5	-.435147E-06	.305479E-07	.715748E-07
4.0	4.0	.0	.000000E-99	.000000E-99	.000000E-99
4.5	2.5	2.5	-.626773E-05	.451107E-06	.103300E-05
4.5	3.5	.5	-.175496E-05	.126310E-06	.289259E-06
5.5	1.5	.5	-.752128E-06	.541328E-07	.123825E-06
4.0	4.0	1.0	-.374823E-05	.270561E-06	.617861E-06
5.0	2.0	2.0	-.374823E-05	.270561E-06	.617564E-06
4.0	3.0	3.0	-.644396E-05	.470442E-06	.106221E-05
5.0	3.0	.0	.000000E-99	.000000E-99	.000000E-99
4.5	3.5	1.5	-.307925E-05	.226630E-06	.507565E-06

TABLE A-XVIII

VALUES OF $\langle \phi_{2s}(0) | \phi_{1s}(\vec{B}) \rangle$, $\langle \phi_{2s}(0) | -\frac{1}{2}\nabla^2 | \phi_{1s}(\vec{B}) \rangle$, $\langle \phi_{2s}(0) | V | \phi_{1s}(\vec{B}) \rangle$ FOR $a_0 = 6.5183$ a.u.

$\vec{B}/a_0$			MULTICENTER INTEGRALS		
$\frac{B_x}{a_0}$	$\frac{B_y}{a_0}$	$\frac{B_z}{a_0}$	OVERLAP	KINETIC ENERGY	POTENTIAL ENERGY
.0	.0	.0	.283891E-03	.682529E 00	-.649664E-00
.5	.5	.5	-.561511E-01	.385883E-03	.955042E-01
1.0	.0	.0	-.369279E-01	.118525E-02	.620334E-01
1.0	1.0	.0	-.900667E-02	.746772E-03	.147518E-01
1.5	.5	.5	-.372288E-02	.379560E-03	.603969E-02
1.0	1.0	1.0	-.283599E-02	.302665E-03	.459020E-02
2.0	.0	.0	-.103826E-02	.125897E-03	.166813E-02
1.5	1.5	.5	-.523589E-03	.675896E-04	.837084E-03
2.0	1.0	.0	-.421188E-03	.553064E-04	.672611E-03
2.0	1.0	1.0	-.184315E-03	.255822E-04	.293276E-03
2.5	.5	.5	-.103155E-03	.147829E-04	.163769E-03
1.5	1.5	1.5	-.103155E-03	.147829E-04	.163785E-03
2.0	2.0	.0	-.416579E-04	.622336E-05	.659462E-04
2.5	1.5	.5	-.249289E-04	.379943E-05	.394066E-04
2.0	2.0	1.0	-.211015E-04	.323558E-05	.333431E-04
3.0	.0	.0	-.211015E-04	.323558E-05	.333400E-04
3.0	1.0	.0	-.110537E-04	.173188E-05	.174377E-04
2.5	1.5	1.5	-.693826E-05	.110234E-05	.109349E-04
3.0	1.0	1.0	-.596045E-05	.951070E-06	.939044E-05
2.0	2.0	2.0	-.329639E-05	.534296E-06	.518767E-05

TABLE A-XVIII (CONT'D)

2.5	2.5	.5	-.214558E-05	.351406E-06	.337383E-05
3.5	.5	.5	-.214558E-05	.351406E-06	.337362E-05
3.0	2.0	.0	-.186429E-05	.306330E-06	.293076E-05
3.0	2.0	1.0	-.107563E-05	.178880E-06	.168947E-05
2.5	2.5	1.5	-.720595E-06	.120815E-06	.113116E-05
3.5	1.5	.5	-.720595E-06	.120815E-06	.113109E-05
4.0	.0	.0	-.377266E-06	.640265E-07	.591621E-06
3.5	1.5	1.5	-.258781E-06	.442081E-07	.405645E-06
3.0	2.0	2.0	-.228627E-06	.391383E-07	.358334E-06
4.0	1.0	.0	-.228627E-06	.391383E-07	.358302E-06
3.0	3.0	.0	-.140449E-06	.242335E-07	.219995E-06
4.0	1.0	1.0	-.140449E-06	.242335E-07	.219986E-06
2.5	2.5	2.5	-.982689E-07	.170482E-07	.153569E-06
3.5	2.5	.5	-.982689E-07	.170482E-07	.153561E-06
3.0	3.0	1.0	-.873704E-07	.151839E-07	.136517E-06
4.0	2.0	.0	-.549857E-07	.961923E-08	.858742E-07
3.5	2.5	1.5	-.391296E-07	.687704E-08	.610951E-07
4.5	.5	.5	-.391296E-07	.687704E-08	.610900E-07
4.0	2.0	1.0	-.349799E-07	.615683E-08	.546089E-07
3.0	3.0	2.0	-.224778E-07	.397874E-08	.350803E-07
4.5	1.5	.5	-.162330E-07	.288480E-08	.253257E-07
4.0	2.0	2.0	-.954161E-08	.170615E-08	.148812E-07
3.5	2.5	2.5	-.698044E-08	.125251E-08	.108847E-07
3.5	3.5	.5	-.698044E-08	.125251E-08	.108843E-07

TABLE A-XIX

VALUES OF $\langle \phi_{2s}(0) | \phi_{2s}(\vec{B}) \rangle$, $\langle \phi_{2s}(0) | -\frac{1}{2}\nabla^2 | \phi_{2s}(\vec{B}) \rangle$,
$\langle \phi_{2s}(0) | V | \phi_{2s}(\vec{B}) \rangle$ FOR $a_0 = 6.5183$ a.u.

$\vec{B}/a_0$			MULTICENTER INTEGRALS		
$\frac{B_x}{a_0}$	$\frac{B_y}{a_0}$	$\frac{B_z}{a_0}$	OVERLAP	KINETIC ENERGY	POTENTIAL ENERGY
.0	.0	.0	.100057E 01	.204844E 00	-.223530E-00
.5	.5	.5	.502777E-00	.169067E-01	-.469490E-01
1.0	.0	.0	.408041E-00	.976562E-02	-.436233E-01
1.0	1.0	.0	.183210E-00	-.132990E-02	-.251471E-01
1.5	.5	.5	.104615E-00	-.250909E-02	-.154704E-01
1.0	1.0	1.0	.874045E-01	-.250701E-02	-.133769E-01
2.0	.0	.0	.439204E-01	-.194888E-02	-.692888E-02
1.5	1.5	.5	.269661E-01	-.144901E-02	-.431780E-02
2.0	1.0	.0	.230281E-01	-.130137E-02	-.369025E-02
2.0	1.0	1.0	.125069E-01	-.828988E-03	-.204345E-02
2.5	.5	.5	.807052E-02	-.584985E-03	-.132895E-02
1.5	1.5	1.5	.807052E-02	-.584985E-03	-.133721E-02
2.0	2.0	.0	.401638E-02	-.326286E-03	-.668067E-03
2.5	1.5	.5	.268776E-02	-.230480E-03	-.448881E-03
2.0	2.0	1.0	.235699E-02	-.205423E-03	-.395082E-03
3.0	.0	.0	.235699E-02	-.205423E-03	-.395269E-03
3.0	1.0	.0	.141051E-02	-.130231E-03	-.237108E-03
2.5	1.5	1.5	.970840E-03	-.930185E-04	-.163996E-03
3.0	1.0	1.0	.858929E-03	-.832368E-04	-.145053E-03
2.0	2.0	2.0	.531286E-03	-.536594E-04	-.902433E-04

TABLE A-XIX (CONT'D)

2.5	2.5	.5	.374042E-03	-.388249E-04	-.634907E-04
3.5	.5	.5	.374042E-03	-.388249E-04	-.635104E-04
3.0	2.0	.0	.333306E-03	-.348924E-04	-.565747E-04
3.0	2.0	1.0	.211814E-03	-.228826E-04	-.360545E-04
2.5	2.5	1.5	.151942E-03	-.167665E-04	-.259249E-04
3.5	1.5	.5	.151942E-03	-.167665E-04	-.258899E-04
4.0	.0	.0	.885436E-04	-.100844E-04	-.151334E-04
3.5	1.5	1.5	.645301E-04	-.747595E-05	-.110357E-04
3.0	2.0	2.0	.581415E-04	-.677235E-05	-.995333E-05
4.0	1.0	.0	.581415E-04	-.677235E-05	-.994440E-05
3.0	3.0	.0	.385364E-04	-.458117E-05	-.659880E-05
4.0	1.0	1.0	.385364E-04	-.458117E-05	-.659957E-05
2.5	2.5	2.5	.284712E-04	-.343268E-05	-.488606E-05
3.5	2.5	.5	.284712E-04	-.343268E-05	-.487871E-05
3.0	3.0	1.0	.257654E-04	-.312046E-05	-.441789E-05
4.0	2.0	.0	.173677E-04	-.213957E-05	-.297935E-05
3.5	2.5	1.5	.129855E-04	-.161886E-05	-.223029E-05
4.5	.5	.5	.129855E-04	-.161886E-05	-.223020E-05
4.0	2.0	1.0	.117968E-04	-.147628E-05	-.202583E-05
3.0	3.0	2.0	.807063E-05	-.102476E-05	-.138804E-05
4.5	1.5	.5	.609826E-05	-.782272E-06	-.104857E-05
4.0	2.0	2.0	.385358E-05	-.502229E-06	-.663339E-06
3.5	2.5	2.5	.293938E-05	-.386501E-06	-.506368E-06
3.5	3.5	.5	.293938E-05	-.386501E-06	-.506061E-06

TABLE A-XIX (CONT'D)

4.5	1.5	1.5	.293938E-05	-.386501E-06	-.506084E-06
4.0	3.0	.0	.268764E-05	-.354414E-06	-.462731E-06
5.0	.0	.0	.268764E-05	-.354414E-06	-.462927E-06
4.0	3.0	1.0	.188530E-05	-.251363E-06	-.324803E-06
5.0	1.0	.0	.188530E-05	-.251363E-06	-.324828E-06
3.5	3.5	1.5	.145029E-05	-.194882E-06	-.250001E-06
4.5	2.5	.5	.145029E-05	-.194882E-06	-.249911E-06
3.0	3.0	3.0	.132974E-05	-.179136E-06	-.229363E-06
5.0	1.0	1.0	.132974E-05	-.179136E-06	-.229208E-06
4.5	2.5	1.5	.730872E-06	-.100117E-06	-.126072E-06
4.0	3.0	2.0	.671806E-06	-.922335E-07	-.115921E-06
5.0	2.0	.0	.671806E-06	-.922335E-07	-.115877E-06
5.0	2.0	1.0	.480982E-06	-.666124E-07	-.829983E-07
3.5	3.5	2.5	.375487E-06	-.523271E-07	-.648427E-07
5.5	.5	.5	.375487E-06	-.523271E-07	-.648227E-07
4.0	4.0	.0	.249890E-06	-.351693E-07	-.431495E-07
4.5	2.5	2.5	.196343E-06	-.277889E-07	-.339192E-07
4.5	3.5	.5	.196343E-06	-.277889E-07	-.339102E-07
5.5	1.5	.5	.196343E-06	-.277889E-07	-.339121E-07
4.0	4.0	1.0	.181270E-06	-.257025E-07	-.313120E-07
5.0	2.0	2.0	.181270E-06	-.257025E-07	-.313126E-07
4.0	3.0	3.0	.132022E-06	-.188531E-07	-.228195E-07
5.0	3.0	.0	.132022E-06	-.188531E-07	-.228081E-07
4.5	3.5	1.5	.104350E-06	-.149778E-07	-.180343E-07

TABLE A-XX

VALUES OF $\langle \phi_{2p_x}(0) \mid \phi_{1s}(\vec{B}) \rangle$, $\langle \phi_{2p_x}(0) \mid -\frac{1}{2}\nabla^2 \mid \phi_{1s}(\vec{B}) \rangle$, $\langle \phi_{2p_x}(0) \mid V \mid \phi_{1s}(\vec{B}) \rangle$ FOR $a_c = 6.5183\ a.u.$

$\vec{B}/a_o$			MULTICENTER INTEGRALS		
$\frac{B_x}{a_o}$	$\frac{B_y}{a_o}$	$\frac{B_z}{a_o}$	OVERLAP	KINETIC ENERGY	POTENTIAL ENERGY
.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
.5	.5	.5	.636346E-01	.355752E-02	-.111642E-00
1.0	.0	.0	.823526E-01	.251517E-02	-.142728E-00
1.0	1.0	.0	.210546E-01	-.380313E-03	-.356436E-01
1.5	.5	.5	.140377E-01	-.496116E-03	-.235672E-01
1.0	1.0	1.0	.732093E-02	-.289869E-03	-.122657E-01
2.0	.0	.0	.598890E-02	-.313706E-03	-.997226E-02
1.5	1.5	.5	.246546E-02	-.145874E-03	-.408825E-02
2.0	1.0	.0	.272007E-02	-.166139E-03	-.450640E-02
2.0	1.0	1.0	.133133E-02	-.898421E-04	-.219923E-02
2.5	.5	.5	.101156E-02	-.721368E-04	-.166807E-02
1.5	1.5	1.5	.606936E-03	-.432821E-04	-.100087E-02
2.0	2.0	.0	.373832E-03	-.285775E-04	-.615065E-03
2.5	1.5	.5	.302525E-03	-.238926E-04	-.497198E-03
2.0	2.0	1.0	.210237E-03	-.167663E-04	-.345412E-03
3.0	.0	.0	.315355E-03	-.251495E-04	-.518099E-03
3.0	1.0	.0	.182928E-03	-.150992E-04	-.300181E-03
2.5	1.5	1.5	.103118E-03	-.870045E-05	-.169090E-03
3.0	1.0	1.0	.108955E-03	-.925478E-05	-.178615E-03
2.0	2.0	2.0	.442674E-04	-.385266E-05	-.725092E-04

TABLE A-XX (CONT'D)

2.5	2.5	.5	.386798E-04	-.342061E-05	-.633202E-04
3.5	.5	.5	.541517E-04	-.478886E-05	-.886463E-04
3.0	2.0	.0	.412900E-04	-.366962E-05	-.675812E-04
3.0	2.0	1.0	.261380E-04	-.236587E-05	-.427540E-04
2.5	2.5	1.5	.156227E-04	-.143155E-05	-.255432E-04
3.5	1.5	.5	.218718E-04	-.200417E-05	-.357598E-04
4.0	.0	.0	.146289E-04	-.136513E-05	-.239023E-04
3.5	1.5	1.5	.937458E-05	-.883427E-06	-.153124E-04
3.0	2.0	2.0	.725419E-05	-.685731E-06	-.118479E-04
4.0	1.0	.0	.967226E-05	-.914308E-06	-.157966E-04
3.0	3.0	.0	.485397E-05	-.464219E-06	-.792449E-05
4.0	1.0	1.0	.647197E-05	-.618959E-06	-.105658E-04
2.5	2.5	2.5	.301437E-05	-.290611E-06	-.491238E-05
3.5	2.5	.5	.422012E-05	-.406856E-06	-.687723E-05
3.0	3.0	1.0	.328377E-05	-.317395E-06	-.535097E-05
4.0	2.0	.0	.299214E-05	-.292023E-06	-.487441E-05
3.5	2.5	1.5	.198007E-05	-.194556E-06	-.322515E-05
4.5	.5	.5	.254581E-05	-.250143E-06	-.414650E-05
4.0	2.0	1.0	.206407E-05	-.203247E-06	-.336174E-05
3.0	3.0	2.0	.107724E-05	-.106949E-06	-.175415E-05
4.5	1.5	.5	.123773E-05	-.123593E-06	-.201516E-05
4.0	2.0	2.0	.712307E-06	-.717642E-07	-.115948E-05
3.5	2.5	2.5	.482768E-06	-.488816E-07	-.785763E-06
3.5	3.5	.5	.482768E-06	-.488816E-07	-.785753E-06

TABLE A-XXI

VALUES OF $\langle \phi_{2P_y}(0) \mid \phi_{1S}(\vec{B}) \rangle$, $\langle \phi_{2P_y}(0) \mid -\frac{1}{2}\nabla^2 \mid \phi_{1S}(\vec{B}) \rangle$, $\langle \phi_{2P_y}(0) \mid V \mid \phi_{1S}(\vec{B}) \rangle$ FOR $a_o = 6.5183$ a.u.

$\vec{B}/a_o$			MULTICENTER INTEGRALS		
$\frac{B_x}{a_o}$	$\frac{B_y}{a_o}$	$\frac{B_z}{a_o}$	OVERLAP	KINETIC ENERGY	POTENTIAL ENERGY
.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
.5	.5	.5	.636346E-01	.355752E-02	-.111642E-00
1.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
1.0	1.0	.0	.210546E-01	-.380313E-03	-.356436E-01
1.5	.5	.5	.467926E-02	-.165372E-03	-.785545E-02
1.0	1.0	1.0	.732093E-02	-.289869E-03	-.122657E-01
2.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
1.5	1.5	.5	.246546E-02	-.145874E-03	-.408825E-02
2.0	1.0	.0	.136003E-02	-.830697E-04	-.225316E-02
2.0	1.0	1.0	.665667E-03	-.449210E-04	-.109959E-02
2.5	.5	.5	.202312E-03	-.144273E-04	-.333607E-03
1.5	1.5	1.5	.606936E-03	-.432821E-04	-.100087E-02
2.0	2.0	.0	.373832E-03	-.285775E-04	-.615065E-03
2.5	1.5	.5	.181515E-03	-.143355E-04	-.298315E-03
2.0	2.0	1.0	.210237E-03	-.167663E-04	-.345412E-03
3.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
3.0	1.0	.0	.609732E-04	-.503308E-05	-.100058E-03
2.5	1.5	1.5	.618713E-04	-.522027E-05	-.101453E-03
3.0	1.0	1.0	.363184E-04	-.308492E-05	-.595376E-04
2.0	2.0	2.0	.442674E-04	-.385266E-05	-.725092E-04

TABLE A-XXI (CONT'D)

2.5	2.5	.5	.386798E-04	-.342061E-05	-.633202E-04
3.5	.5	.5	.773596E-05	-.684123E-06	-.126635E-04
3.0	2.0	.0	.275267E-04	-.244641E-05	-.450538E-04
3.0	2.0	1.0	.174253E-04	-.157724E-05	-.285024E-04
2.5	2.5	1.5	.156227E-04	-.143155E-05	-.255432E-04
3.5	1.5	.5	.937363E-05	-.858933E-06	-.153254E-04
4.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
3.5	1.5	1.5	.401768E-05	-.378611E-06	-.656241E-05
3.0	2.0	2.0	.483613E-05	-.457154E-06	-.789855E-05
4.0	1.0	.0	.241806E-05	-.228577E-06	-.394911E-05
3.0	3.0	.0	.485397E-05	-.464219E-06	-.792449E-05
4.0	1.0	1.0	.161799E-05	-.154739E-06	-.264142E-05
2.5	2.5	2.5	.301437E-05	-.290611E-06	-.491238E-05
3.5	2.5	.5	.301437E-05	-.290611E-06	-.491228E-05
3.0	3.0	1.0	.328377E-05	-.317395E-06	-.535097E-05
4.0	2.0	.0	.149607E-05	-.146011E-06	-.243718E-05
3.5	2.5	1.5	.141434E-05	-.138968E-06	-.230367E-05
4.5	.5	.5	.282868E-06	-.277937E-07	-.460716E-06
4.0	2.0	1.0	.103203E-05	-.101623E-06	-.168085E-05
3.0	3.0	2.0	.107724E-05	-.106949E-06	-.175415E-05
4.5	1.5	.5	.412579E-06	-.411977E-07	-.671714E-06
4.0	2.0	2.0	.356153E-06	-.358821E-07	-.579739E-06
3.5	2.5	2.5	.344834E-06	-.349154E-07	-.561257E-06
3.5	3.5	.5	.482768E-06	-.488816E-07	-.785753E-06

TABLE A-XXII

VALUES OF $\langle \phi_{2p_z}(0) \mid \phi_{1s}(\vec{B}) \rangle$, $\langle \phi_{2p_z}(0) \mid -\frac{1}{2}\nabla^2 \mid \phi_{1s}(\vec{B}) \rangle$, $\langle \phi_{2p_z}(0) \mid V \mid \phi_{1s}(\vec{B}) \rangle$ FOR $a_o = 6.5183\ au$

$\vec{B}/a_o$			MULTICENTER INTEGRALS		
$\frac{B_x}{a_o}$	$\frac{B_y}{a_o}$	$\frac{B_z}{a_o}$	OVERLAP	KINETIC ENERGY	POTENTIAL ENERGY
.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
.5	.5	.5	.636346E-01	.355752E-02	-.111642E-00
1.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
1.0	1.0	.0	.000000E-99	.000000E-99	.000000E-99
1.5	.5	.5	.467926E-02	-.165372E-03	-.785545E-02
1.0	1.0	1.0	.732093E-02	-.289869E-03	-.122657E-01
2.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
1.5	1.5	.5	.821822E-03	-.486247E-04	-.136271E-02
2.0	1.0	.0	.000000E-99	.000000E-99	.000000E-99
2.0	1.0	1.0	.665667E-03	-.449210E-04	-.109959E-02
2.5	.5	.5	.202312E-03	-.144273E-04	-.333607E-03
1.5	1.5	1.5	.606936E-03	-.432821E-04	-.100087E-02
2.0	2.0	.0	.000000E-99	.000000E-99	.000000E-99
2.5	1.5	.5	.605051E-04	-.477852E-05	-.994373E-04
2.0	2.0	1.0	.105118E-03	-.838317E-05	-.172703E-03
3.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
3.0	1.0	.0	.000000E-99	.000000E-99	.000000E-99
2.5	1.5	1.5	.618713E-04	-.522027E-05	-.101453E-03
3.0	1.0	1.0	.363184E-04	-.308492E-05	-.595376E-04
2.0	2.0	2.0	.442674E-04	-.385266E-05	-.725092E-04

TABLE A-XXII (CONT'D)

2.5	2.5	.5	.773596E-05	-.684123E-06	-.126638E-04
3.5	.5	.5	.773596E-05	-.684123E-06	-.126635E-04
3.0	2.0	.0	.000000E-99	.000000E-99	.000000E-99
3.0	2.0	1.0	.871266E-05	-.788623E-06	-.142511E-04
2.5	2.5	1.5	.937363E-05	-.858933E-06	-.153258E-04
3.5	1.5	.5	.312454E-05	-.286311E-06	-.510846E-05
4.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
3.5	1.5	1.5	.401768E-05	-.378611E-06	-.656241E-05
3.0	2.0	2.0	.483613E-05	-.457154E-06	-.789855E-05
4.0	1.0	.0	.000000E-99	.000000E-99	.000000E-99
3.0	3.0	.0	.000000E-99	.000000E-99	.000000E-99
4.0	1.0	1.0	.161799E-05	-.154739E-06	-.264142E-05
2.5	2.5	2.5	.301437E-05	-.290611E-06	-.491238E-05
3.5	2.5	.5	.602874E-06	-.581223E-07	-.982447E-06
3.0	3.0	1.0	.109459E-05	-.105798E-06	-.178363E-05
4.0	2.0	.0	.000000E-99	.000000E-99	.000000E-99
3.5	2.5	1.5	.848604E-06	-.833812E-07	-.138219E-05
4.5	.5	.5	.282868E-06	-.277937E-07	-.460716E-06
4.0	2.0	1.0	.516018E-06	-.508118E-07	-.840425E-06
3.0	3.0	2.0	.718160E-06	-.712997E-07	-.116943E-05
4.5	1.5	.5	.137526E-06	-.137325E-07	-.223904E-06
4.0	2.0	2.0	.356153E-06	-.358821E-07	-.579739E-06
3.5	2.5	2.5	.344834E-06	-.349154E-07	-.561257E-06
3.5	3.5	.5	.689668E-07	-.698309E-08	-.112249E-06

TABLE A-XXIII

VALUES OF $\langle \phi_{2P_x}(0) \mid \phi_{2s}(\vec{B}) \rangle$, $\langle \phi_{2P_x}(0) \mid -\frac{1}{2}\nabla^2 \mid \phi_{2s}(\vec{B}) \rangle$, $\langle \phi_{2P_x}(0) \mid V \mid \phi_{2s}(\vec{B}) \rangle$ FOR $a_o = 6.5183$ au

$\vec{B}/a_o$			MULTICENTER INTEGRALS		
$\frac{B_x}{a_o}$	$\frac{B_y}{a_o}$	$\frac{B_z}{a_o}$	OVERLAP	KINETIC ENERGY	POTENTIAL ENERGY
.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
.5	.5	.5	-.318250E-00	-.235410E-01	.307347E-01
1.0	.0	.0	-.511709E-00	-.315604E-01	.558371E-01
1.0	1.0	.0	-.227607E-00	-.609715E-02	.312085E-01
1.5	.5	.5	-.197194E-00	-.192569E-02	.288606E-01
1.0	1.0	1.0	-.110482E-00	-.566554E-03	.167285E-01
2.0	.0	.0	-.114436E-00	.114098E-02	.177306E-01
1.5	1.5	.5	-.541582E-01	.101405E-02	.850435E-02
2.0	1.0	.0	-.622692E-01	.132552E-02	.978375E-02
2.0	1.0	1.0	-.352398E-01	.106372E-02	.564170E-02
2.5	.5	.5	-.293643E-01	.104949E-02	.473390E-02
1.5	1.5	1.5	-.176186E-01	.629698E-03	.285687E-02
2.0	2.0	.0	-.123666E-01	.537459E-03	.201283E-02
2.5	1.5	.5	-.107077E-01	.507379E-03	.175012E-02
2.0	2.0	1.0	-.759951E-02	.369307E-03	.124376E-02
3.0	.0	.0	-.113992E-01	.553961E-03	.186528E-02
3.0	1.0	.0	-.714749E-02	.379056E-03	.117316E-02
2.5	1.5	1.5	-.424650E-02	.237768E-03	.700418E-03
3.0	1.0	1.0	-.456173E-02	.259637E-03	.752146E-03
2.0	2.0	2.0	-.197181E-02	.119000E-03	.326948E-03

TABLE A-XXIII (CONT'D)

2.5	2.5	.5	-.179769E-02	.112680E-03	.298013E-03
3.5	.5	.5	-.251677E-02	.157752E-03	.417257E-03
3.0	2.0	.0	-.194506E-02	.123347E-03	.322497E-03
3.0	2.0	1.0	-.129562E-02	.857336E-04	.215471E-03
2.5	2.5	1.5	-.802243E-03	.546050E-04	.133740E-03
3.5	1.5	.5	-.112314E-02	.764470E-04	.186985E-03
4.0	.0	.0	-.793021E-03	.562564E-04	.132410E-03
3.5	1.5	1.5	-.523669E-03	.379744E-04	.875370E-04
3.0	2.0	2.0	-.409143E-03	.298754E-04	.684701E-04
4.0	1.0	.0	-.545524E-03	.398338E-04	.911933E-04
3.0	3.0	.0	-.284025E-03	.212827E-04	.475464E-04
4.0	1.0	1.0	-.378701E-03	.283769E-04	.633991E-04
2.5	2.5	2.5	-.181013E-03	.138058E-04	.303723E-04
3.5	2.5	.5	-.253419E-03	.193282E-04	.424636E-04
3.0	3.0	1.0	-.198843E-03	.152510E-04	.333408E-04
4.0	2.0	.0	-.187078E-03	.146549E-04	.313884E-04
3.5	2.5	1.5	-.126640E-03	.100664E-04	.212793E-04
4.5	.5	.5	-.162823E-03	.129425E-04	.273491E-04
4.0	2.0	1.0	-.132983E-03	.106198E-04	.223407E-04
3.0	3.0	2.0	-.713889E-04	.580244E-05	.120140E-04
4.5	1.5	.5	-.836878E-04	.688618E-05	.140803E-04
4.0	2.0	2.0	-.497070E-04	.416817E-05	.837547E-05
3.5	2.5	2.5	-.342983E-04	.290645E-05	.578472E-05
3.5	3.5	.5	-.342983E-04	.290645E-05	.578020E-05

TABLE A-XXIV

VALUES OF $\langle \phi_{2P_y}(0) \mid \phi_{2s}(\vec{B}) \rangle$, $\langle \phi_{2P_y}(0) \mid -\frac{1}{2}\nabla^2 \mid \phi_{2s}(\vec{B}) \rangle$, $\langle \phi_{2P_y}(0) \mid V \mid \phi_{2s}(\vec{B}) \rangle$ FOR $a_o = 6.5183\ au$

$\vec{B}/a_o$			MULTICENTER INTEGRALS		
$\frac{B_x}{a_o}$	$\frac{B_y}{a_o}$	$\frac{B_z}{a_o}$	OVERLAP	KINETIC ENERGY	POTENTIAL ENERGY
.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
.5	.5	.5	-.318250E-00	-.235410E-01	.307347E-01
1.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
1.0	1.0	.0	-.227607E-00	-.609715E-02	.312085E-01
1.5	.5	.5	-.657314E-01	-.641897E-03	.964757E-02
1.0	1.0	1.0	-.110482E-00	-.566554E-03	.167285E-01
2.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
1.5	1.5	.5	-.541582E-01	.101405E-02	.850435E-02
2.0	1.0	.0	-.311346E-01	.662763E-03	.489244E-02
2.0	1.0	1.0	-.176199E-01	.531860E-03	.282284E-02
2.5	.5	.5	-.587287E-02	.209899E-03	.946815E-03
1.5	1.5	1.5	-.176186E-01	.629698E-03	.285687E-02
2.0	2.0	.0	-.123666E-01	.537459E-03	.201283E-02
2.5	1.5	.5	-.642463E-02	.304427E-03	.105011E-02
2.0	2.0	1.0	-.759951E-02	.369307E-03	.124376E-02
3.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
3.0	1.0	.0	-.238249E-02	.126352E-03	.391091E-03
2.5	1.5	1.5	-.254790E-02	.142660E-03	.420214E-03
3.0	1.0	1.0	-.152057E-02	.865459E-04	.250711E-03
2.0	2.0	2.0	-.197181E-02	.119000E-03	.326948E-03

TABLE A-XXIV (CONT'D)

2.5	2.5	.5	-.179769E-02	.112680E-03	.298013E-03
3.5	.5	.5	-.359539E-03	.225360E-04	.596173E-04
3.0	2.0	.0	-.129671E-02	.822317E-04	.214992E-03
3.0	2.0	1.0	-.863749E-03	.571557E-04	.143638E-03
2.5	2.5	1.5	-.802243E-03	.546050E-04	.133740E-03
3.5	1.5	.5	-.481345E-03	.327630E-04	.801389E-04
4.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
3.5	1.5	1.5	-.224429E-03	.162747E-04	.375098E-04
3.0	2.0	2.0	-.272762E-03	.199169E-04	.456383E-04
4.0	1.0	.0	-.136381E-03	.995847E-05	.228021E-04
3.0	3.0	.0	-.284025E-03	.212827E-04	.475464E-04
4.0	1.0	1.0	-.946752E-04	.709423E-05	.158496E-04
2.5	2.5	2.5	-.181013E-03	.138058E-04	.303723E-04
3.5	2.5	.5	-.181013E-03	.138058E-04	.303298E-04
3.0	3.0	1.0	-.198843E-03	.152510E-04	.333408E-04
4.0	2.0	.0	-.935392E-04	.732749E-05	.156943E-04
3.5	2.5	1.5	-.904575E-04	.719030E-05	.151981E-04
4.5	.5	.5	-.180915E-04	.143806E-05	.303930E-05
4.0	2.0	1.0	-.664915E-04	.530993E-05	.111698E-04
3.0	3.0	2.0	-.713889E-04	.580244E-05	.120140E-04
4.5	1.5	.5	-.278959E-04	.229539E-05	.469373E-05
4.0	2.0	2.0	-.248535E-04	.208408E-05	.418698E-05
3.5	2.5	2.5	-.244988E-04	.207604E-05	.413133E-05
3.5	3.5	.5	-.342983E-04	.290645E-05	.578020E-05

TABLE A-XXV

VALUES OF $\langle \phi_{2p_z}(0) \mid \phi_{2s}(\vec{B}) \rangle$, $\langle \phi_{2p_z}(0) \mid -\frac{1}{2}\nabla^2 \mid \phi_{2s}(\vec{B}) \rangle$, $\langle \phi_{2p_z}(0) \mid V \mid \phi_{2s}(\vec{B}) \rangle$ FOR $a_0 = 6.5183\,au$

$\vec{B}/a_0$			MULTICENTER INTEGRALS		
$\frac{B_x}{a_0}$	$\frac{B_y}{a_0}$	$\frac{B_z}{a_0}$	OVERLAP	KINETIC ENERGY	POTENTIAL ENERGY
.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
.5	.5	.5	-.318250E-00	-.235410E-01	.307347E-01
1.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
1.0	1.0	.0	.000000E-99	.000000E-99	.000000E-99
1.5	.5	.5	-.657314E-01	-.641897E-03	.964757E-02
1.0	1.0	1.0	-.110482E-00	-.566554E-03	.167285E-01
2.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
1.5	1.5	.5	-.180527E-01	.338018E-03	.284240E-02
2.0	1.0	.0	.000000E-99	.000000E-99	.000000E-99
2.0	1.0	1.0	-.176199E-01	.531860E-03	.282284E-02
2.5	.5	.5	-.587287E-02	.209899E-03	.946815E-03
1.5	1.5	1.5	-.176186E-01	.629698E-03	.285687E-02
2.0	2.0	.0	.000000E-99	.000000E-99	.000000E-99
2.5	1.5	.5	-.214154E-02	.101475E-03	.350074E-03
2.0	2.0	1.0	-.379975E-02	.184653E-03	.621919E-03
3.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
3.0	1.0	.0	.000000E-99	.000000E-99	.000000E-99
2.5	1.5	1.5	-.254790E-02	.142660E-03	.420214E-03
3.0	1.0	1.0	-.152057E-02	.865459E-04	.250711E-03
2.0	2.0	2.0	-.197181E-02	.119000E-03	.326948E-03

TABLE A-XXV (CONT'D)

2.5	2.5	.5	-.359539E-03	.225360E-04	.595839E-04
3.5	.5	.5	-.359539E-03	.225360E-04	.596173E-04
3.0	2.0	.0	.000000E-99	.000000E-99	.000000E-99
3.0	2.0	1.0	-.431874E-03	.285778E-04	.718016E-04
2.5	2.5	1.5	-.481345E-03	.327630E-04	.802239E-04
3.5	1.5	.5	-.160448E-03	.109210E-04	.267066E-04
4.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
3.5	1.5	1.5	-.224429E-03	.162747E-04	.375098E-04
3.0	2.0	2.0	-.272762E-03	.199169E-04	.456383E-04
4.0	1.0	.0	.000000E-99	.000000E-99	.000000E-99
3.0	3.0	.0	.000000E-99	.000000E-99	.000000E-99
4.0	1.0	1.0	-.946752E-04	.709423E-05	.158496E-04
2.5	2.5	2.5	-.181013E-03	.138058E-04	.303723E-04
3.5	2.5	.5	-.362027E-04	.276117E-05	.606375E-05
3.0	3.0	1.0	-.662810E-04	.508367E-05	.111093E-04
4.0	2.0	.0	.000000E-99	.000000E-99	.000000E-99
3.5	2.5	1.5	-.542745E-04	.431418E-05	.911677E-05
4.5	.5	.5	-.180915E-04	.143806E-05	.303930E-05
4.0	2.0	1.0	-.332457E-04	.265496E-05	.558370E-05
3.0	3.0	2.0	-.475926E-04	.386829E-05	.800765E-05
4.5	1.5	.5	-.929864E-05	.765131E-06	.156430E-05
4.0	2.0	2.0	-.248535E-04	.208408E-05	.418698E-05
3.5	2.5	2.5	-.244988E-04	.207604E-05	.413133E-05
3.5	3.5	.5	-.489976E-05	.415208E-06	.825417E-06

TABLE A-XXVI

VALUES OF $\langle \phi_{2p_x}(0) | \phi_{2p_x}(\vec{B}) \rangle$, $\langle \phi_{2p_x}(0) | -\frac{1}{2}\nabla^2 | \phi_{2p_x}(\vec{B}) \rangle$, $\langle \phi_{2p_x}(0) | V | \phi_{2p_x}(\vec{B}) \rangle$ FOR $a_0 = 6.5183\ au$

$\vec{B}/a_0$			MULTICENTER INTEGRALS		
$\frac{B_x}{a_0}$	$\frac{B_y}{a_0}$	$\frac{B_z}{a_0}$	OVERLAP	KINETIC ENERGY	POTENTIAL ENERGY
.0	.0	.0	.999119E 00	.140902E-00	-.159464E-00
.5	.5	.5	.273580E-00	.662987E-02	-.458672E-01
1.0	.0	.0	-.241597E-00	-.442179E-01	.319862E-01
1.0	1.0	.0	-.692074E-01	-.980021E-02	.107824E-01
1.5	.5	.5	-.207075E-00	-.108480E-01	.343293E-01
1.0	1.0	1.0	-.218480E-01	-.297912E-02	.421308E-02
2.0	.0	.0	-.188299E-00	-.420533E-02	.322205E-01
1.5	1.5	.5	-.497726E-01	-.959440E-03	.854071E-02
2.0	1.0	.0	-.998086E-01	-.971041E-03	.169992E-01
2.0	1.0	1.0	-.554700E-01	.211258E-05	.952746E-02
2.5	.5	.5	-.646489E-01	.517862E-03	.111288E-01
1.5	1.5	1.5	-.147970E-01	-.656192E-05	.259614E-02
2.0	2.0	.0	-.190377E-01	.275151E-03	.328606E-02
2.5	1.5	.5	-.235338E-01	.482218E-03	.405883E-02
2.0	2.0	1.0	-.116191E-01	.232383E-03	.201310E-02
3.0	.0	.0	-.322127E-01	.727165E-03	.557252E-02
3.0	1.0	.0	-.203146E-01	.554423E-03	.351034E-02
2.5	1.5	1.5	-.938469E-02	.278686E-03	.162519E-02
3.0	1.0	1.0	-.130542E-01	.410208E-03	.225811E-02
2.0	2.0	2.0	-.298052E-02	.974232E-04	.519080E-03

TABLE A-XXVI (CONT'D)

2.5	2.5	.5	-.401009E-02	.147836E-03	.694838E-03
3.5	.5	.5	-.891545E-02	.338286E-03	.154453E-02
3.0	2.0	.0	-.565464E-02	.216886E-03	.978873E-03
3.0	2.0	1.0	-.379900E-02	.156922E-03	.658284E-03
2.5	2.5	1.5	-.181010E-02	.772282E-04	.314314E-03
3.5	1.5	.5	-.406050E-02	.177416E-03	.703552E-03
4.0	.0	.0	-.342612E-02	.160971E-03	.594355E-03
3.5	1.5	1.5	-.193364E-02	.937335E-04	.335339E-03
3.0	2.0	2.0	-.123264E-02	.600058E-04	.213979E-03
4.0	1.0	.0	-.238412E-02	.117345E-03	.413503E-03
3.0	3.0	.0	-.863666E-03	.438355E-04	.149840E-03
4.0	1.0	1.0	-.167425E-02	.858607E-04	.290429E-03
2.5	2.5	2.5	-.419046E-03	.216147E-04	.728868E-04
3.5	2.5	.5	-.955978E-03	.502238E-04	.165833E-03
3.0	3.0	1.0	-.610299E-03	.321493E-04	.105939E-03
4.0	2.0	.0	-.846355E-03	.465283E-04	.146836E-03
3.5	2.5	1.5	-.488040E-03	.273521E-04	.847236E-04
4.5	.5	.5	-.855797E-03	.482257E-04	.148554E-03
4.0	2.0	1.0	-.608550E-03	.344660E-04	.105607E-03
3.0	3.0	2.0	-.225307E-03	.130004E-04	.391528E-04
4.5	1.5	.5	-.450413E-03	.267603E-04	.781867E-04
4.0	2.0	2.0	-.235298E-03	.143602E-04	.408580E-04
3.5	2.5	2.5	-.137842E-03	.852371E-05	.239499E-04
3.5	3.5	.5	-.137842E-03	.852371E-05	.239370E-04

TABLE A-XXVI (CONT'D)

4.5	1.5	1.5	-.242933E-03	.150918E-04	.421801E-04
4.0	3.0	.0	-.173461E-03	.108116E-04	.301168E-04
5.0	.0	.0	-.283124E-03	.177002E-04	.491718E-04
4.0	3.0	1.0	-.128563E-03	.817127E-05	.223262E-04
5.0	1.0	.0	-.210009E-03	.133867E-04	.364719E-04
3.5	3.5	1.5	-.758013E-04	.487160E-05	.131692E-04
4.5	2.5	.5	-.133913E-03	.864363E-05	.232532E-04
3.0	3.0	3.0	-.484880E-04	.311608E-05	.843180E-05
5.0	1.0	1.0	-.156567E-03	.101621E-04	.271916E-04
4.5	2.5	1.5	-.752752E-04	.502313E-05	.130746E-04
4.0	3.0	2.0	-.539111E-04	.360573E-05	.936659E-05
5.0	2.0	.0	-.882678E-04	.591926E-05	.153303E-04
5.0	2.0	1.0	-.667174E-04	.454088E-05	.115884E-04
3.5	3.5	2.5	-.242667E-04	.166100E-05	.421833E-05
5.5	.5	.5	-.665707E-04	.458223E-05	.115653E-04
4.0	4.0	.0	-.235159E-04	.164047E-05	.408543E-05
4.5	2.5	2.5	-.250413E-04	.176596E-05	.435108E-05
4.5	3.5	.5	-.250413E-04	.176596E-05	.435031E-05
5.5	1.5	.5	-.387454E-04	.273693E-05	.673125E-05

TABLE A-XXVII

VALUES OF $\langle \phi_{2P_y}(0) | \phi_{2P_y}(\vec{B}) \rangle$, $\langle \phi_{2P_y}(0) | -\frac{1}{2}\nabla^2 | \phi_{2P_y}(\vec{B}) \rangle$, $\langle \phi_{2P_y}(0) | V | \phi_{2P_y}(\vec{B}) \rangle$ FOR $a_o = 6.5183$ a.u.

$\vec{B}/a_o$			MULTICENTER INTEGRALS		
$\frac{B_x}{a_o}$	$\frac{B_y}{a_o}$	$\frac{B_z}{a_o}$	OVERLAP	KINETIC ENERGY	POTENTIAL ENERGY
.0	.0	.0	.999119E 00	.140902E-00	-.159464E-00
.5	.5	.5	.273580E-00	.662987E-02	-.458672E-01
1.0	.0	.0	.389151E-00	.219447E-01	-.642027E-01
1.0	1.0	.0	-.692074E-01	-.980021E-02	.107824E-01
1.5	.5	.5	.776725E-01	.227471E-03	-.133642E-01
1.0	1.0	1.0	-.218480E-01	-.297912E-02	.421308E-02
2.0	.0	.0	.540155E-01	-.867401E-04	-.920116E-02
1.5	1.5	.5	-.497726E-01	-.959440E-03	.854071E-02
2.0	1.0	.0	-.135100E-02	-.497886E-03	.169274E-03
2.0	1.0	1.0	.371729E-03	-.257776E-03	-.507885E-04
2.5	.5	.5	.101288E-01	-.268774E-03	-.175116E-02
1.5	1.5	1.5	-.147970E-01	-.656192E-05	.259614E-02
2.0	2.0	.0	-.190377E-01	.275151E-03	.328606E-02
2.5	1.5	.5	-.501503E-02	.608232E-04	.864781E-03
2.0	2.0	1.0	-.116191E-01	.232383E-03	.201310E-02
3.0	.0	.0	.485571E-02	-.163442E-03	-.838170E-03
3.0	1.0	.0	.590736E-03	-.451652E-04	-.103992E-03
2.5	1.5	1.5	-.186199E-02	.395671E-04	.324827E-03
3.0	1.0	1.0	.457658E-03	-.324179E-04	-.792737E-04
2.0	2.0	2.0	-.298052E-02	.974232E-04	.519080E-03

TABLE A-XXVII (CONT'D)

2.5	2.5	.5	-.401009E-02	.147836E-03	.694838E-03
3.5	.5	.5	.898265E-03	-.426146E-04	-.155222E-03
3.0	2.0	.0	-.195627E-02	.704286E-04	.338747E-03
3.0	2.0	1.0	-.130130E-02	.507357E-04	.225781E-03
2.5	2.5	1.5	-.181010E-02	.772282E-04	.314314E-03
3.5	1.5	.5	-.309841E-03	.104356E-04	.536079E-04
4.0	.0	.0	.346766E-03	-.185275E-04	-.601198E-04
3.5	1.5	1.5	-.135289E-03	.515014E-05	.235369E-04
3.0	2.0	2.0	-.410154E-03	.190491E-04	.713806E-04
4.0	1.0	.0	.833387E-04	-.552476E-05	-.144969E-04
3.0	3.0	.0	-.863666E-03	.438355E-04	.149840E-03
4.0	1.0	1.0	.627244E-04	-.419319E-05	-.108959E-04
2.5	2.5	2.5	-.419046E-03	.216147E-04	.728868E-04
3.5	2.5	.5	-.419046E-03	.216147E-04	.727197E-04
3.0	3.0	1.0	-.610299E-03	.321493E-04	.105939E-03
4.0	2.0	.0	-.140617E-03	.735182E-05	.243921E-04
3.5	2.5	1.5	-.212223E-03	.116970E-04	.368730E-04
4.5	.5	.5	.635945E-04	-.395816E-05	-.110415E-04
4.0	2.0	1.0	-.999614E-04	.539441E-05	.173565E-04
3.0	3.0	2.0	-.225307E-03	.130004E-04	.391528E-04
4.5	1.5	.5	-.134387E-04	.627700E-06	.232928E-05
4.0	2.0	2.0	-.373685E-04	.218262E-05	.649902E-05
3.5	2.5	2.5	-.590244E-04	.359762E-05	.102667E-04
3.5	3.5	.5	-.137842E-03	.852371E-05	.239370E-04

TABLE A-XXVII (CONT'D)

4.5	1.5	1.5	-.647905E-05	.313562E-06	.112618E-05
4.0	3.0	.0	-.881674E-04	.545392E-05	.153109E-04
5.0	.0	.0	.214959E-04	-.143461E-05	-.373270E-05
4.0	3.0	1.0	-.652171E-04	.411480E-05	.113290E-04
5.0	1.0	.0	.717894E-05	-.521154E-06	-.124767E-05
3.5	3.5	1.5	-.758013E-04	.487160E-05	.131692E-04
4.5	2.5	.5	-.322173E-04	.204258E-05	.559531E-05
3.0	3.0	3.0	-.484880E-04	.311608E-05	.843180E-05
5.0	1.0	1.0	.555185E-05	-.406966E-06	-.964843E-06
4.5	2.5	1.5	-.179360E-04	.117671E-05	.311708E-05
4.0	3.0	2.0	-.271892E-04	.180632E-05	.472625E-05
5.0	2.0	.0	-.810225E-05	.521029E-06	.140687E-05
5.0	2.0	1.0	-.605294E-05	.395349E-06	.105151E-05
3.5	3.5	2.5	-.242667E-04	.166100E-05	.421833E-05
5.5	.5	.5	.393597E-05	-.286485E-06	-.683856E-06
4.0	4.0	.0	-.235159E-04	.164047E-05	.408543E-05
4.5	2.5	2.5	-.585568E-05	.406589E-06	.101836E-05
4.5	3.5	.5	-.140781E-04	.989176E-06	.244606E-05
5.5	1.5	.5	-.374060E-06	.181975E-07	.648665E-07

TABLE A-XXVIII

VALUES OF $\langle \phi_{2p_z}(0) \mid \phi_{2p_z}(\vec{B}) \rangle$, $\langle \phi_{2p_z}(0) \mid -\frac{1}{2}\nabla^2 \mid \phi_{2p_z}(\vec{B}) \rangle$, $\langle \phi_{2p_z}(0) \mid V \mid \phi_{2p_z}(\vec{B}) \rangle$ FOR $a_0 = 6.5183 au$

$\vec{B}/a_0$			MULTICENTER INTEGRALS		
$\frac{B_x}{a_0}$	$\frac{B_y}{a_0}$	$\frac{B_z}{a_0}$	OVERLAP	KINETIC ENERGY	POTENTIAL ENERGY
.0	.0	.0	.999119E 00	.140902E-00	-.159464E-00
.5	.5	.5	.273580E-00	.662987E-02	-.458672E-01
1.0	.0	.0	.389151E-00	.219447E-01	-.642027E-01
1.0	1.0	.0	.185268E-00	.515233E-02	-.327558E-01
1.5	.5	.5	.776725E-01	.227471E-03	-.133642E-01
1.0	1.0	1.0	-.218480E-01	-.297912E-02	.421308E-02
2.0	.0	.0	.540155E-01	-.867401E-04	-.920116E-02
1.5	1.5	.5	.263716E-01	-.384621E-03	-.460163E-02
2.0	1.0	.0	.314682E-01	-.340168E-03	-.547934E-02
2.0	1.0	1.0	.371729E-03	-.257776E-03	-.507885E-04
2.5	.5	.5	.101288E-01	-.268774E-03	-.175116E-02
1.5	1.5	1.5	-.147970E-01	-.656192E-05	.259614E-02
2.0	2.0	.0	.748858E-02	-.219226E-03	-.130690E-02
2.5	1.5	.5	.424438E-02	-.149874E-03	-.738504E-03
2.0	2.0	1.0	.736998E-03	-.644864E-04	-.126157E-03
3.0	.0	.0	.485571E-02	-.163442E-03	-.838170E-03
3.0	1.0	.0	.320391E-02	-.120113E-03	-.556299E-03
2.5	1.5	1.5	-.186199E-02	.395671E-04	.324827E-03
3.0	1.0	1.0	.457658E-03	-.324179E-04	-.792737E-04
2.0	2.0	2.0	-.298052E-02	.974232E-04	.519080E-03

TABLE A-XXVIII (CONT'D)

2.5	2.5	.5	.895265E-03	-.426146E-04	-.155902E-03
3.5	.5	.5	.895265E-03	-.426146E-04	-.155222E-03
3.0	2.0	.0	.100241E-02	-.467375E-04	-.174520E-03
3.0	2.0	1.0	.197306E-03	-.129760E-04	-.342286E-04
2.5	2.5	1.5	-.309841E-03	.104356E-04	.541070E-04
3.5	1.5	.5	.440290E-03	-.229605E-04	-.765294E-04
4.0	.0	.0	.346766E-03	-.185275E-04	-.601198E-04
3.5	1.5	1.5	-.135289E-03	.515014E-05	.235369E-04
3.0	2.0	2.0	-.410154E-03	.190491E-04	.713806E-04
4.0	1.0	.0	.247836E-03	-.137160E-04	-.430384E-04
3.0	3.0	.0	.178523E-03	-.101967E-04	-.310813E-04
4.0	1.0	1.0	.627244E-04	-.419319E-05	-.108959E-04
2.5	2.5	2.5	-.419046E-03	.216147E-04	.728868E-04
3.5	2.5	.5	.117886E-03	-.699431E-05	-.205130E-04
3.0	3.0	1.0	.473305E-04	-.319453E-05	-.822602E-05
4.0	2.0	.0	.946281E-04	-.570701E-05	-.164576E-04
3.5	2.5	1.5	-.283446E-04	.126022E-05	.494156E-05
4.5	.5	.5	.635945E-04	-.395816E-05	-.110415E-04
4.0	2.0	1.0	.271857E-04	-.187349E-05	-.472445E-05
3.0	3.0	2.0	-.715533E-04	.397405E-05	.124580E-04
4.5	1.5	.5	.351140E-04	-.227592E-05	-.610275E-05
4.0	2.0	2.0	-.373685E-04	.218262E-05	.649902E-05
3.5	2.5	2.5	-.590244E-04	.359762E-05	.102667E-04
3.5	3.5	.5	.197936E-04	-.132846E-05	-.344432E-05

TABLE A-XXVIII (CONT'D)

4.5	1.5	1.5	-.647905E-05	.313562E-06	.112618E-05
4.0	3.0	.0	.214959E-04	-.143461E-05	-.374039E-05
5.0	.0	.0	.214959E-04	-.143461E-05	-.373270E-05
4.0	3.0	1.0	.717894E-05	-.521154E-06	-.124833E-05
5.0	1.0	.0	.162284E-04	-.110064E-05	-.281950E-05
3.5	3.5	1.5	-.316135E-05	.156566E-06	.551242E-06
4.5	2.5	.5	.113666E-04	-.786440E-06	-.197695E-05
3.0	3.0	3.0	-.484880E-04	.311608E-05	.843180E-05
5.0	1.0	1.0	.555185E-05	-.406966E-06	-.964843E-06
4.5	2.5	1.5	-.155348E-05	.777428E-07	.270556E-06
4.0	3.0	2.0	-.810225E-05	.521029E-06	.141004E-05
5.0	2.0	.0	.716738E-05	-.507206E-06	-.124618E-05
5.0	2.0	1.0	.261340E-05	-.196870E-06	-.454319E-06
3.5	3.5	2.5	-.101653E-04	.687258E-06	.176860E-05
5.5	.5	.5	.393597E-05	-.286485E-06	-.683856E-06
4.0	4.0	.0	.327829E-05	-.240392E-06	-.570405E-06
4.5	2.5	2.5	-.585568E-05	.406589E-06	.101836E-05
4.5	3.5	.5	.236675E-05	-.175998E-06	-.411741E-06
5.5	1.5	.5	.236675E-05	-.175998E-06	-.411389E-06

TABLE XXIX

VALUES OF $\langle \phi_{2P_y}(0) | \phi_{2P_x}(\vec{B}) \rangle$, $\langle \phi_{2P_y}(0) | -\frac{1}{2}\nabla^2 | \phi_{2P_x}(\vec{B}) \rangle$, $\langle \phi_{2P_y}(0) | V | \phi_{2P_x}(\vec{B}) \rangle$ FOR $a_0 = 6.5183$ a.u.

$\vec{B}/a_0$			MULTICENTER INTEGRALS		
$\frac{B_x}{a_0}$	$\frac{B_y}{a_0}$	$\frac{B_z}{a_0}$	OVERLAP	KINETIC ENERGY	POTENTIAL ENERGY
.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
.5	.5	.5	-.205726E-00	-.256612E-01	.297748E-01
1.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
1.0	1.0	.0	-.254475E-00	-.149525E-01	.415284E-01
1.5	.5	.5	-.106780E-00	-.415331E-02	.181384E-01
1.0	1.0	1.0	-.118840E-00	-.400010E-02	.203291E-01
2.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
1.5	1.5	.5	-.856623E-01	-.646670E-03	.146445E-01
2.0	1.0	.0	-.656384E-01	-.315436E-03	.112337E-01
2.0	1.0	1.0	-.372278E-01	.173259E-03	.642804E-02
2.5	.5	.5	-.155787E-01	.163882E-03	.268818E-02
1.5	1.5	1.5	-.280416E-01	.294988E-03	.485632E-02
2.0	2.0	.0	-.265262E-01	.494377E-03	.457398E-02
2.5	1.5	.5	-.173614E-01	.395058E-03	.299865E-02
2.0	2.0	1.0	-.164748E-01	.395825E-03	.284863E-02
3.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
3.0	1.0	.0	-.783952E-02	.224845E-03	.135556E-02
2.5	1.5	1.5	-.705252E-02	.224174E-03	.122290E-02
3.0	1.0	1.0	-.506697E-02	.165984E-03	.878030E-03
2.0	2.0	2.0	-.443851E-02	.161429E-03	.770495E-03

TABLE A-XXIX (CONT'D)

2.5	2.5	.5	-.510975E-02	.198386E-03	.884963E-03
3.5	.5	.5	-.143073E-02	.555481E-04	.247953E-03
3.0	2.0	.0	-.443803E-02	.175749E-03	.768639E-03
3.0	2.0	1.0	-.299723E-02	.127423E-03	.519614E-03
2.5	2.5	1.5	-.234416E-02	.104363E-03	.406683E-03
3.5	1.5	.5	-.196909E-02	.876651E-04	.341362E-03
4.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
3.5	1.5	1.5	-.944139E-03	.465063E-04	.163893E-03
3.0	2.0	2.0	-.986986E-03	.491479E-04	.171399E-03
4.0	1.0	.0	-.657990E-03	.327652E-04	.114134E-03
3.0	3.0	.0	-.104219E-02	.540323E-04	.180781E-03
4.0	1.0	1.0	-.463195E-03	.240143E-04	.803960E-04
2.5	2.5	2.5	-.559304E-03	.298011E-04	.971738E-04
3.5	2.5	.5	-.783026E-03	.417215E-04	.135857E-03
3.0	3.0	1.0	-.739834E-03	.397618E-04	.128390E-03
4.0	2.0	.0	-.470491E-03	.261176E-04	.816482E-04
3.5	2.5	1.5	-.402233E-03	.228304E-04	.698411E-04
4.5	.5	.5	-.103431E-03	.587068E-05	.179556E-04
4.0	2.0	1.0	-.339059E-03	.193810E-04	.588622E-04
3.0	3.0	2.0	-.276757E-03	.162475E-04	.480725E-04
4.5	1.5	.5	-.163865E-03	.979974E-05	.284506E-04
4.0	2.0	2.0	-.131953E-03	.811842E-05	.229245E-04
3.5	2.5	2.5	-.114943E-03	.718388E-05	.199737E-04
3.5	3.5	.5	-.160920E-03	.100574E-04	.279419E-04

TABLE A-XXIX (CONT'D)

4.5	1.5	1.5	-.886703E-04	.554185E-05	.154028E-04
4.0	3.0	.0	-.146217E-03	.918472E-05	.253889E-04
5.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
4.0	3.0	1.0	-.108594E-03	.695394E-05	.188600E-04
5.0	1.0	.0	-.452475E-04	.289747E-05	.785824E-05
3.5	3.5	1.5	-.889839E-04	.577592E-05	.154570E-04
4.5	2.5	.5	-.817199E-04	.530441E-05	.141925E-04
3.0	3.0	3.0	-.607949E-04	.396342E-05	.105667E-04
5.0	1.0	1.0	-.337749E-04	.220190E-05	.586707E-05
4.5	2.5	1.5	-.460760E-04	.309086E-05	.800490E-05
4.0	3.0	2.0	-.458089E-04	.308470E-05	.795956E-05
5.0	2.0	.0	-.381740E-04	.257058E-05	.663085E-05
5.0	2.0	1.0	-.288878E-04	.197406E-05	.501864E-05
3.5	3.5	2.5	-.287902E-04	.198806E-05	.500351E-05
5.5	.5	.5	-.646311E-05	.446299E-06	.112285E-05
4.0	4.0	.0	-.267942E-04	.188086E-05	.465475E-05
4.5	2.5	2.5	-.154170E-04	.109235E-05	.267955E-05
4.5	3.5	.5	-.215839E-04	.152929E-05	.374982E-05
5.5	1.5	.5	-.113058E-04	.801057E-06	.196432E-05
4.0	4.0	1.0	-.205185E-04	.145820E-05	.356493E-05
5.0	2.0	2.0	-.128240E-04	.911375E-06	.222866E-05
4.0	3.0	3.0	-.118272E-04	.850407E-06	.205590E-05
5.0	3.0	.0	-.147841E-04	.106300E-05	.256861E-05

TABLE A-XXX

VALUES OF $\langle \phi_{2p_z}(0) \mid \phi_{2p_x}(\vec{B}) \rangle$, $\langle \phi_{2p_z}(0) \mid -\frac{1}{2}\nabla^2 \mid \phi_{2p_x}(\vec{B}) \rangle$, $\langle \phi_{2p_z}(0) \mid V \mid \phi_{2p_x}(\vec{B}) \rangle$ FOR $a_0 = 6.5183\, a.u.$

$\vec{B}/a_0$			MULTICENTER INTEGRALS		
$\frac{B_x}{a_0}$	$\frac{B_y}{a_0}$	$\frac{B_z}{a_0}$	OVERLAP	KINETIC ENERGY	POTENTIAL ENERGY
.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
.5	.5	.5	-.205726E-00	-.256612E-01	.297748E-01
1.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
1.0	1.0	.0	.000000E-99	.000000E-99	.000000E-99
1.5	.5	.5	-.106780E-00	-.415331E-02	.181384E-01
1.0	1.0	1.0	-.118840E-00	-.400010E-02	.203291E-01
2.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
1.5	1.5	.5	-.285541E-01	-.215556E-03	.493345E-02
2.0	1.0	.0	.000000E-99	.000000E-99	.000000E-99
2.0	1.0	1.0	-.372278E-01	.173259E-03	.642804E-02
2.5	.5	.5	-.155787E-01	.163882E-03	.268818E-02
1.5	1.5	1.5	-.280416E-01	.294988E-03	.485632E-02
2.0	2.0	.0	.000000E-99	.000000E-99	.000000E-99
2.5	1.5	.5	-.578713E-02	.131686E-03	.100298E-02
2.0	2.0	1.0	-.823744E-02	.197912E-03	.142896E-02
3.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
3.0	1.0	.0	.000000E-99	.000000E-99	.000000E-99
2.5	1.5	1.5	-.705252E-02	.224174E-03	.122290E-02
3.0	1.0	1.0	-.506697E-02	.165984E-03	.878030E-03
2.0	2.0	2.0	-.443851E-02	.161429E-03	.770495E-03

TABLE A-XXX (CONT'D)

2.5	2.5	.5	-.102195E-02	.396772E-04	.177465E-03
3.5	.5	.5	-.143073E-02	.555481E-04	.247953E-03
3.0	2.0	.0	.000000E-99	.000000E-99	.000000E-99
3.0	2.0	1.0	-.149861E-02	.637117E-04	.260201E-03
2.5	2.5	1.5	-.140649E-02	.626179E-04	.244303E-03
3.5	1.5	.5	-.656365E-03	.292217E-04	.113923E-03
4.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
3.5	1.5	1.5	-.944139E-03	.465063E-04	.163893E-03
3.0	2.0	2.0	-.986986E-03	.491479E-04	.171399E-03
4.0	1.0	.0	.000000E-99	.000000E-99	.000000E-99
3.0	3.0	.0	.000000E-99	.000000E-99	.000000E-99
4.0	1.0	1.0	-.463195E-03	.240143E-04	.803960E-04
2.5	2.5	2.5	-.559304E-03	.298011E-04	.971738E-04
3.5	2.5	.5	-.156605E-03	.834431E-05	.272093E-04
3.0	3.0	1.0	-.246611E-03	.132539E-04	.428529E-04
4.0	2.0	.0	.000000E-99	.000000E-99	.000000E-99
3.5	2.5	1.5	-.241340E-03	.136982E-04	.419344E-04
4.5	.5	.5	-.103431E-03	.587068E-05	.179556E-04
4.0	2.0	1.0	-.169529E-03	.969054E-05	.294504E-04
3.0	3.0	2.0	-.184504E-03	.108316E-04	.320651E-04
4.5	1.5	.5	-.546219E-04	.326658E-05	.948779E-05
4.0	2.0	2.0	-.131953E-03	.811842E-05	.229245E-04
3.5	2.5	2.5	-.114943E-03	.718388E-05	.199737E-04
3.5	3.5	.5	-.229886E-04	.143677E-05	.399578E-05

TABLE A-XXX (CONT'D)

4.5	1.5	1.5	-.886703E-04	.554185E-05	.154028E-04
4.0	3.0	.0	.000000E-99	.000000E-99	.000000E-99
5.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
4.0	3.0	1.0	-.361980E-04	.231798E-05	.629165E-05
5.0	1.0	.0	.000000E-99	.000000E-99	.000000E-99
3.5	3.5	1.5	-.381359E-04	.247539E-05	.662899E-05
4.5	2.5	.5	-.163439E-04	.106088E-05	.284044E-05
3.0	3.0	3.0	-.607949E-04	.396342E-05	.105667E-04
5.0	1.0	1.0	-.337749E-04	.220190E-05	.586707E-05
4.5	2.5	1.5	-.276456E-04	.185452E-05	.480470E-05
4.0	3.0	2.0	-.305392E-04	.205647E-05	.530829E-05
5.0	2.0	.0	.000000E-99	.000000E-99	.000000E-99
5.0	2.0	1.0	-.144439E-04	.987032E-06	.251006E-05
3.5	3.5	2.5	-.205644E-04	.142004E-05	.357488E-05
5.5	.5	.5	-.646311E-05	.446299E-06	.112285E-05
4.0	4.0	.0	.000000E-99	.000000E-99	.000000E-99
4.5	2.5	2.5	-.154170E-04	.109235E-05	.267955E-05
4.5	3.5	.5	-.308341E-05	.218470E-06	.536038E-06
5.5	1.5	.5	-.376861E-05	.267019E-06	.654895E-06
4.0	4.0	1.0	-.512962E-05	.364550E-06	.891788E-06
5.0	2.0	2.0	-.128240E-04	.911375E-06	.222866E-05
4.0	3.0	3.0	-.118272E-04	.850407E-06	.205590E-05
5.0	3.0	.0	.000000E-99	.000000E-99	.000000E-99

TABLE A-XXXI

VALUES OF $\langle \phi_{2p_z}(0) | \phi_{2p_y}(\vec{B}) \rangle$, $\langle \phi_{2p_z}(0) | -\frac{1}{2}\nabla^2 | \phi_{2p_y}(\vec{B}) \rangle$, $\langle \phi_{2p_z}(0) | V | \phi_{2p_y}(\vec{B}) \rangle$ FOR $a_o = 6.5183$ au

$\vec{B}/a_o$			MULTICENTER INTEGRALS		
B_x/a_o	B_y/a_o	B_z/a_o	OVERLAP	KINETIC ENERGY	POTENTIAL ENERGY
.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
.5	.5	.5	-.205726E-00	-.256612E-01	.297748E-01
1.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
1.0	1.0	.0	.000000E-99	.000000E-99	.000000E-99
1.5	.5	.5	-.355935E-01	-.138443E-02	.564435E-02
1.0	1.0	1.0	-.118840E-00	-.400010E-02	.203291E-01
2.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
1.5	1.5	.5	-.285541E-01	-.215556E-03	.493345E-02
2.0	1.0	.0	.000000E-99	.000000E-99	.000000E-99
2.0	1.0	1.0	-.186139E-01	.866297E-04	.319501E-02
2.5	.5	.5	-.311574E-02	.327765E-04	.523620E-03
1.5	1.5	1.5	-.280416E-01	.294988E-03	.485632E-02
2.0	2.0	.0	.000000E-99	.000000E-99	.000000E-99
2.5	1.5	.5	-.347228E-02	.790116E-04	.600252E-03
2.0	2.0	1.0	-.823744E-02	.197912E-03	.142896E-02
3.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
3.0	1.0	.0	.000000E-99	.000000E-99	.000000E-99
2.5	1.5	1.5	-.423151E-02	.134504E-03	.733472E-03
3.0	1.0	1.0	-.168899E-02	.553282E-04	.291526E-03
2.0	2.0	2.0	-.443851E-02	.161429E-03	.770495E-03

TABLE A-XXXI (CONT'D)

2.5	2.5	.5	-.102195E-02	.396772E-04	.177465E-03
3.5	.5	.5	-.204390E-03	.793544E-05	.351128E-04
3.0	2.0	.0	.000000E-99	.000000E-99	.000000E-99
3.0	2.0	1.0	-.999077E-03	.424745E-04	.173370E-03
2.5	2.5	1.5	-.140649E-02	.626179E-04	.244303E-03
3.5	1.5	.5	-.281299E-03	.125235E-04	.487229E-04
4.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
3.5	1.5	1.5	-.404631E-03	.199312E-04	.701974E-04
3.0	2.0	2.0	-.657990E-03	.327652E-04	.114288E-03
4.0	1.0	.0	.000000E-99	.000000E-99	.000000E-99
3.0	3.0	.0	.000000E-99	.000000E-99	.000000E-99
4.0	1.0	1.0	-.115798E-03	.600359E-05	.200582E-04
2.5	2.5	2.5	-.559304E-03	.298011E-04	.971738E-04
3.5	2.5	.5	-.111860E-03	.596022E-05	.194290E-04
3.0	3.0	1.0	-.246611E-03	.132539E-04	.428529E-04
4.0	2.0	.0	.000000E-99	.000000E-99	.000000E-99
3.5	2.5	1.5	-.172385E-03	.978448E-05	.299506E-04
4.5	.5	.5	-.114923E-04	.652298E-06	.198892E-05
4.0	2.0	1.0	-.847647E-04	.484527E-05	.147165E-04
3.0	3.0	2.0	-.184504E-03	.108316E-04	.320651E-04
4.5	1.5	.5	-.182073E-04	.108886E-05	.315868E-05
4.0	2.0	2.0	-.659766E-04	.405921E-05	.114624E-04
3.5	2.5	2.5	-.821021E-04	.513134E-05	.142696E-04
3.5	3.5	.5	-.229886E-04	.143677E-05	.399578E-05

TABLE A-XXXI (CONT'D)

4.5	1.5	1.5	-.295567E-04	.184728E-05	.513178E-05
4.0	3.0	.0	.000000E-99	.000000E-99	.000000E-99
5.0	.0	.0	.000000E-99	.000000E-99	.000000E-99
4.0	3.0	1.0	-.271485E-04	.173848E-05	.471826E-05
5.0	1.0	.0	.000000E-99	.000000E-99	.000000E-99
3.5	3.5	1.5	-.381359E-04	.247539E-05	.662899E-05
4.5	2.5	.5	-.907999E-05	.589379E-06	.157747E-05
3.0	3.0	3.0	-.607949E-04	.396342E-05	.105667E-04
5.0	1.0	1.0	-.675499E-05	.440380E-06	.117221E-05
4.5	2.5	1.5	-.153586E-04	.103028E-05	.266890E-05
4.0	3.0	2.0	-.229044E-04	.154235E-05	.398131E-05
5.0	2.0	.0	.000000E-99	.000000E-99	.000000E-99
5.0	2.0	1.0	-.577756E-05	.394813E-06	.100358E-05
3.5	3.5	2.5	-.205644E-04	.142004E-05	.357488E-05
5.5	.5	.5	-.587556E-06	.405726E-07	.101951E-06
4.0	4.0	.0	.000000E-99	.000000E-99	.000000E-99
4.5	2.5	2.5	-.856504E-05	.606862E-06	.148881E-05
4.5	3.5	.5	-.239821E-05	.169921E-06	.416890E-06
5.5	1.5	.5	-.102780E-05	.728234E-07	.178484E-06
4.0	4.0	1.0	-.512962E-05	.364550E-06	.891788E-06
5.0	2.0	2.0	-.512962E-05	.364550E-06	.891403E-06
4.0	3.0	3.0	-.887046E-05	.637805E-06	.154212E-05
5.0	3.0	.0	.000000E-99	.000000E-99	.000000E-99