Tight-Binding Method for Hexagonal Close-Packed Structure

MARIA MIĄSEK
Institute of Theoretical Physics, University of Warsaw, Warsaw, Poland
(Received March 27, 1957)

Tables for reduction of the matrix components of energy in the tight-binding approximation have been prepared for the hexagonal close-packed lattice.

THE tight-binding or LCAO method has been thoroughly discussed by Slater and Koster[1] in application to cubic lattices. They have given detailed tables of the matrix components of energy in terms of three- and subsequently two-center integrals. Analogous tables for a hexagonal lattice are more tedious to construct in view of the more complicated symmetry of this lattice, the directions along the axes of a rectangular coordinate system being nonequivalent. Moreover, only the close-packed hexagonal lattice exists in nature and this is the lattice with basis.

The element to which the tight-binding method could be applied is the hexagonal cobalt, α-Co. Cobalt belongs to the group of transition elements, the d states of which can be treated with the tight-binding approximation.

There are in the literature a few papers on energy bands in hexagonal structures,[2,3] and in particular Schiff has given the symmetry properties needed for the cellular method.

The hexagonal close-packed lattice can be regarded as the simple hexagonal lattice with two atoms in the unit cell. The primitive translation vectors in a rectangular coordinate system are: $\mathbf{A}_1=(\frac{1}{2}a, -\frac{1}{2}\sqrt{3}a, 0)$, $\mathbf{A}_2=(\frac{1}{2}a, \frac{1}{2}\sqrt{3}a, 0)$, $\mathbf{A}_3=(0,0,c)$. Basis vectors are given by $\mathbf{t}_1=(0,0,0)$ and $\mathbf{t}_2=(\frac{1}{2}a, \frac{1}{6}\sqrt{3}a, \frac{1}{2}c)$. The simple hexagonal lattice which has an atom in position (0,0,0) is denoted by 1, and the simple lattice with the atom in position $(\frac{1}{2}a, \frac{1}{6}\sqrt{3}a, \frac{1}{2}c)$ is denoted by 2. It is convenient to use different length units along the different axes of the rectangular coordinate system. So we take $\alpha=\frac{1}{2}a$, $\beta=\frac{1}{2}\sqrt{3}a$, $\gamma=\frac{1}{2}c$ in the x, y, z directions, respectively. In the calculations we used the model of a hexagonal ideal close-packed lattice, i.e., we assumed $|\mathbf{t}_2|=a$.

TABLE I. Relations among the matrix components of energy for states of various symmetries.

$(s,s)_{11}=(s/s)_{22}$	$(s/s)_{12}=(s/s)_{21}^*$
$(s/p_j)_{11}=-(s/p_j)_{22}^*$	$(s/p_j)_{12}=-(s/p_j)_{21}^*$
$(s/d_q)_{11}=(s/d_q)_{22}^*$	$(s/d_q)_{12}=(s/d_q)_{21}^*$
$(p_j/p_j)_{11}=(p_j/p_j)_{22}$	$(p_j/p_j)_{12}=(p_j/p_j)_{21}^*$
$(p_j/p_i)_{11}=(p_j/p_i)_{22}^*$	$(p_j/p_i)_{12}=(p_j/p_i)_{21}^*,\ j\neq i$
$(p_j/d_q)_{11}=-(p_j/d_q)_{22}^*$	$(p_j/d_q)_{12}=-(p_j/d_q)_{21}^*$
$(d_q/d_q)_{11}=(d_q/d_q)_{22}$	$(d_q/d_q)_{12}=(d_q/d_q)_{21}^*$
$(d_q/d_r)_{11}=(d_q/d_r)_{22}^*$	$(d_q/d_r)_{12}=(d_q/d_r)_{21}^*,\ q\neq r$

[1] J. C. Slater and G. F. Koster, Phys. Rev. **94**, 1498 (1954).
[2] C. Herring and A. G. Hill, Phys. Rev. **58**, 132 (1940).
[3] B. Schiff, Proc. Roy. Soc. (London) **A68**, 686 (1955).

The matrix components of energy have been calculated for states of the following symmetries: s, p [3 functions of type x, y, z times $f_1(r)$ denoted by p_j] and d [5 functions of type xy, yz, xz, x^2-y^2, $3z^2-r^2$ times $f_2(r)$ denoted by d_q]. There are nine such states, and a unit cell contains two nonequivalent atoms, so we construct 18 Bloch sums.

The general formula for the matrix component is

$$(m/n)_{\omega'\omega}=\exp[i\mathbf{k}\cdot(\mathbf{t}_\omega-\mathbf{t}_{\omega'})]\sum_i \exp(i\mathbf{k}\cdot\mathbf{r}_i)\times\int \varphi_m^*(\mathbf{r}-\mathbf{t}_{\omega'})H\varphi_n(\mathbf{r}-\mathbf{r}_i-\mathbf{t}_\omega)d\mathbf{r}.$$

Here m and n distinguish the electronic states, the φ_n denote atomic functions, the $\mathbf{r}_i$ are translation vectors, and the $\mathbf{t}_\omega$ are basis vectors.

The energy integrals (E integrals) have the form

$$E_{m,n}(\mathbf{t}_{\omega'}, \mathbf{r}_i+\mathbf{t}_\omega)=\int \varphi_m^*(\mathbf{r}-\mathbf{t}_{\omega'})H\varphi_n(\mathbf{r}-\mathbf{r}_i-\mathbf{t}_\omega)d\mathbf{r}.$$

First of all, by virtue of the symmetry and Hermitian properties of the Hamiltonian and of the symmetries of the atomic functions, we notice that only 90 of the total of 324 matrix components must be considered. We calculate 45 components of the type

$$(m/n)_{11}=\sum_i \exp(i\mathbf{k}\cdot\mathbf{r}_i)\int \varphi_m^*(\mathbf{r})H\varphi_n(\mathbf{r}-\mathbf{r}_i)d\mathbf{r}=(n/m)_{11}^*$$

and 45 components of type

$$(m/n)_{12}=\sum_i \exp[i\mathbf{k}\cdot(\mathbf{r}_i+\mathbf{t}_2)]\times\int \varphi_m^*(\mathbf{r})H\varphi_n(\mathbf{r}-\mathbf{r}_i-\mathbf{t}_2)d\mathbf{r}=(n/m)_{21}^*.$$

Further relations are given in Table I.

We now make the nearest-neighbors approximation. In the hexagonal ideal close-packed lattice every atom has 12 nearest neighbors. So we have in $(m/n)_{11}$ seven E integrals for lattice sites: (0,0,0), (1, −1, 0), (1,1,0), (−1, 1, 0), (−2, 0, 0), (−1, −1, 0), (2,0,0) in terms of α, β, γ; and in $(m/n)_{12}$ we have six E integrals for lattice sites $\mathbf{r}_i+\mathbf{t}_2$: $(1,\frac{1}{3},1)$, $(-1,\frac{1}{3},1)$, $(0,-\frac{2}{3},1)$, $(1,\frac{1}{3},-1)$, $(-1,\frac{1}{3},-1)$, $(0,-\frac{2}{3},-1)$. So 585 E integrals remain to be calculated. Not all of them are independent. Taking into account further particular symmetries, we see that nonvanishing E integrals in $(m/n)_{11}$ can be expressed in terms of E integrals in-

TABLE II. Matrix components of energy expressed in terms of E integrals.

$(s/z)_{11}=(s/yz)_{11}=(s/xz)_{11}=(x/z)_{11}=(x/yz)_{11}=(x/xz)_{11}=(y/z)_{11}=(y/yz)_{11}=(y/xz)_{11}=(z/xy)_{11}=(z/x^2-y^2)_{11}=(z/3z^2-r^2)_{11}=(xy/yz)_{11}=(xy/xz)_{11}=(yz/x^2-y^2)_{11}=(yz/3z^2-r^2)_{11}=(xz/x^2-y^2)_{11}=(xz/3z^2-r^2)_{11}=0$

$(s/s)_{11}$	$E_{s,s}(0)+2E_{s,s}(\mathrm{R})(2\cos\xi\cos\eta+\cos2\xi)$
$(s/s)_{12}$	$2E_{s,s}(\mathrm{T})\cos\zeta[(2\cos\xi\cos\frac{1}{3}\eta+\cos\frac{2}{3}\eta)+i(2\cos\xi\sin\frac{1}{3}\eta-\sin\frac{2}{3}\eta)]$
$(s/x)_{11}$	$-2\sqrt{3}E_{s,y}(\mathrm{R})\sin\xi\sin\eta+2iE_{s,x}(\mathrm{R})(\sin\xi\cos\eta+\sin2\xi)$
$(s/x)_{12}$	$2\sqrt{3}E_{s,y}(\mathrm{T})\sin\xi\cos\zeta(\sin\frac{1}{3}\eta-i\cos\frac{1}{3}\eta)$
$(s/y)_{11}$	$E_{s,y}(0)-2E_{s,y}(\mathrm{R})(\cos\xi\cos\eta-\cos2\xi)+2\sqrt{3}iE_{s,x}(\mathrm{R})\cos\xi\sin\eta$
$(s/y)_{12}$	$-2E_{s,y}(\mathrm{T})\cos\zeta[(\cos\xi\cos\frac{1}{3}\eta-\cos\frac{2}{3}\eta)+i(\cos\xi\sin\frac{1}{3}\eta+\sin\frac{2}{3}\eta)]$
$(s/z)_{12}$	$-2E_{s,z}(\mathrm{T})\sin\zeta[(2\cos\xi\sin\frac{1}{3}\eta-\sin\frac{2}{3}\eta)-i(2\cos\xi\cos\frac{1}{3}\eta+\cos\frac{2}{3}\eta)]$
$(s/xy)_{11}$	$-2\sqrt{3}E_{s,x^2-y^2}(\mathrm{R})\sin\xi\sin\eta+2iE_{s,xy}(\mathrm{R})(\sin\xi\cos\eta+\sin2\xi)$
$(s/xy)_{12}$	$2\sqrt{3}E_{s,x^2-y^2}(\mathrm{T})\sin\xi\cos\zeta(\sin\frac{1}{3}\eta-i\cos\frac{1}{3}\eta)$
$(s/yz)_{12}$	$2E_{s,yz}(\mathrm{T})\sin\zeta[(\cos\xi\sin\frac{1}{3}\eta+\sin\frac{2}{3}\eta)-i(\cos\xi\cos\frac{1}{3}\eta-\cos\frac{2}{3}\eta)]$
$(s/xz)_{12}$	$2\sqrt{3}E_{s,yz}(\mathrm{T})\sin\xi\sin\zeta(\cos\frac{1}{3}\eta+i\sin\frac{1}{3}\eta)$
$(s/x^2-y^2)_{11}$	$E_{s,x^2-y^2}(0)-2E_{s,x^2-y^2}(\mathrm{R})(\cos\xi\cos\eta-\cos2\xi)+2\sqrt{3}iE_{s,xy}(\mathrm{R})\cos\xi\sin\eta$
$(s/x^2-y^2)_{12}$	$-2E_{s,x^2-y^2}(\mathrm{T})\cos\zeta[(\cos\xi\cos\frac{1}{3}\eta-\cos\frac{2}{3}\eta)+i(\cos\xi\sin\frac{1}{3}\eta+\sin\frac{2}{3}\eta)]$
$(s/3z^2-r^2)_{11}$	$E_{s,3z^2-r^2}(0)+2E_{s,3z^2-r^2}(\mathrm{R})(2\cos\xi\cos\eta+\cos2\xi)$
$(s/3z^2-r^2)_{12}$	$2E_{s,3z^2-r^2}(\mathrm{T})\cos\zeta[(2\cos\xi\cos\frac{1}{3}\eta+\cos\frac{2}{3}\eta)+i(2\cos\xi\sin\frac{1}{3}\eta-\sin\frac{2}{3}\eta)]$
$(x/x)_{11}$	$E_{x,x}(0)+[E_{x,x}(\mathrm{R})+3E_{y,y}(\mathrm{R})]\cos\xi\cos\eta+2E_{x,x}(\mathrm{R})\cos2\xi$
$(x/x)_{12}$	$\cos\zeta\{[E_{x,x}(\mathrm{T})+3E_{y,y}(\mathrm{T})]\cos\xi\cos\frac{1}{3}\eta+2E_{x,x}(\mathrm{T})\cos\frac{2}{3}\eta\}+i\cos\zeta\{[E_{x,x}(\mathrm{T})+3E_{y,y}(\mathrm{T})]\cos\xi\sin\frac{1}{3}\eta-2E_{x,x}(\mathrm{T})\sin\frac{2}{3}\eta\}$
$(x/y)_{11}$	$\sqrt{3}[E_{y,y}(\mathrm{R})-E_{x,x}(\mathrm{R})]\sin\xi\sin\eta-2iE_{x,y}(\mathrm{R})(2\sin\xi\cos\eta-\sin2\xi)$
$(x/y)_{12}$	$\sqrt{3}[E_{x,x}(\mathrm{T})-E_{y,y}(\mathrm{T})]\sin\xi\cos\zeta(\sin\frac{1}{3}\eta-i\cos\frac{1}{3}\eta)$
$(x/z)_{12}$	$2\sqrt{3}E_{y,z}(\mathrm{T})\sin\xi\sin\zeta(\cos\frac{1}{3}\eta+i\sin\frac{1}{3}\eta)$
$(x/xy)_{11}$	$E_{x,xy}(0)+[E_{x,xy}(\mathrm{R})+3E_{y,x^2-y^2}(\mathrm{R})]\cos\xi\cos\eta+2E_{x,xy}(\mathrm{R})\cos2\xi+\sqrt{3}i[E_{x,x^2-y^2}(\mathrm{R})+E_{y,xy}(\mathrm{R})]\cos\xi\sin\eta$
$(x/xy)_{12}$	$\cos\zeta\{[E_{x,xy}(\mathrm{T})+3E_{y,x^2-y^2}(\mathrm{T})]\cos\xi\cos\frac{1}{3}\eta+2E_{x,xy}(\mathrm{T})\cos\frac{2}{3}\eta\}+i\cos\zeta\{[E_{x,xy}(\mathrm{T})+3E_{y,x^2-y^2}(\mathrm{T})]\cos\xi\sin\frac{1}{3}\eta-2E_{x,xy}(\mathrm{T})\sin\frac{2}{3}\eta\}$
$(x/yz)_{12}=(y/xz)_{12}$	$\sqrt{3}[E_{x,xz}(\mathrm{T})-E_{y,yz}(\mathrm{T})]\sin\xi\sin\zeta(\cos\frac{1}{3}\eta+i\sin\frac{1}{3}\eta)$
$(x/xz)_{12}$	$\sin\zeta\{-[E_{x,xz}(\mathrm{T})+3E_{y,yz}(\mathrm{T})]\cos\xi\sin\frac{1}{3}\eta+2E_{x,xz}(\mathrm{T})\sin\frac{2}{3}\eta\}+i\sin\zeta\{[E_{x,xz}(\mathrm{T})+3E_{y,yz}(\mathrm{T})]\cos\xi\cos\frac{1}{3}\eta+2E_{x,xz}(\mathrm{T})\cos\frac{2}{3}\eta\}$
$(x/x^2-y^2)_{11}$	$\sqrt{3}[E_{y,x^2-y^2}(\mathrm{R})-E_{x,xy}(\mathrm{R})]\sin\xi\sin\eta-i\{[E_{x,x^2-y^2}(\mathrm{R})-3E_{y,xy}(\mathrm{R})]\sin\xi\cos\eta-2E_{x,x^2-y^2}(\mathrm{R})\sin2\xi\}$
$(x/x^2-y^2)_{12}=(y/xy)_{12}$	$\sqrt{3}[E_{x,xy}(\mathrm{T})-E_{y,x^2-y^2}(\mathrm{T})]\sin\xi\cos\zeta(\sin\frac{1}{3}\eta-i\cos\frac{1}{3}\eta)$
$(x/3z^2-r^2)_{11}$	$-2\sqrt{3}E_{y,3z^2-r^2}(\mathrm{R})\sin\xi\sin\eta+2iE_{x,3z^2-r^2}(\mathrm{R})(\sin\xi\cos\eta+\sin2\xi)$
$(x/3z^2-r^2)_{12}$	$2\sqrt{3}E_{y,3z^2-r^2}(\mathrm{T})\sin\xi\cos\zeta(\sin\frac{1}{3}\eta-i\cos\frac{1}{3}\eta)$
$(y/y)_{11}$	$E_{y,y}(0)+[E_{y,y}(\mathrm{R})+3E_{x,x}(\mathrm{R})]\cos\xi\cos\eta+2E_{y,y}(\mathrm{R})\cos2\xi$
$(y/y)_{12}$	$\cos\zeta\{[E_{y,y}(\mathrm{T})+3E_{x,x}(\mathrm{T})]\cos\xi\cos\frac{1}{3}\eta+2E_{y,y}(\mathrm{T})\cos\frac{2}{3}\eta\}+i\cos\zeta\{[E_{y,y}(\mathrm{T})+3E_{x,x}(\mathrm{T})]\cos\xi\sin\frac{1}{3}\eta-2E_{y,y}(\mathrm{T})\sin\frac{2}{3}\eta\}$
$(y/z)_{12}$	$2E_{y,z}(\mathrm{T})\sin\zeta[(\cos\xi\sin\frac{1}{3}\eta+\sin\frac{2}{3}\eta)-i(\cos\xi\cos\frac{1}{3}\eta-\cos\frac{2}{3}\eta)]$
$(y/xy)_{11}$	$\sqrt{3}[E_{y,x^2-y^2}(\mathrm{R})-E_{x,xy}(\mathrm{R})]\sin\xi\sin\eta-i\{[E_{y,xy}(\mathrm{R})-3E_{x,x^2-y^2}(\mathrm{R})]\sin\xi\cos\eta-2E_{y,xy}(\mathrm{R})\sin2\xi\}$
$(y/yz)_{12}$	$\sin\zeta\{-[E_{y,yz}(\mathrm{T})+3E_{x,xz}(\mathrm{T})]\cos\xi\sin\frac{1}{3}\eta+2E_{y,yz}(\mathrm{T})\sin\frac{2}{3}\eta\}+i\sin\zeta\{[E_{y,yz}(\mathrm{T})+3E_{x,xz}(\mathrm{T})]\cos\xi\cos\frac{1}{3}\eta+2E_{y,yz}(\mathrm{T})\cos\frac{2}{3}\eta\}$
$(y/x^2-y^2)_{11}$	$E_{y,x^2-y^2}(0)+[E_{y,x^2-y^2}(\mathrm{R})+3E_{x,xy}(\mathrm{R})]\cos\xi\cos\eta+2E_{y,x^2-y^2}(\mathrm{R})\cos2\xi-\sqrt{3}i[E_{x,x^2-y^2}(\mathrm{R})+E_{y,xy}(\mathrm{R})]\cos\xi\sin\eta$
$(y/x^2-y^2)_{12}$	$\cos\zeta\{[E_{y,x^2-y^2}(\mathrm{T})+3E_{x,xy}(\mathrm{T})]\cos\xi\cos\frac{1}{3}\eta+2E_{y,x^2-y^2}(\mathrm{T})\cos\frac{2}{3}\eta\}+i\cos\zeta\{[E_{y,x^2-y^2}(\mathrm{T})+3E_{x,xy}(\mathrm{T})]\cos\xi\sin\frac{1}{3}\eta-2E_{y,x^2-y^2}(\mathrm{T})\sin\frac{2}{3}\eta\}$
$(y/3z^2-r^2)_{11}$	$E_{y,3z^2-r^2}(0)-2E_{y,3z^2-r^2}(\mathrm{R})(\cos\xi\cos\eta-\cos2\xi)+2\sqrt{3}iE_{x,3z^2-r^2}(\mathrm{R})\cos\xi\sin\eta$
$(y/3z^2-r^2)_{12}$	$-2E_{y,3z^2-r^2}(\mathrm{T})\cos\zeta[(\cos\xi\cos\frac{1}{3}\eta-\cos\frac{2}{3}\eta)+i(\cos\xi\sin\frac{1}{3}\eta+\sin\frac{2}{3}\eta)]$
$(z/z)_{11}$	$E_{z,z}(0)+2E_{z,z}(\mathrm{R})(2\cos\xi\cos\eta+\cos2\xi)$
$(z/z)_{12}$	$2E_{z,z}(\mathrm{T})\cos\zeta[(2\cos\xi\cos\frac{1}{3}\eta+\cos\frac{2}{3}\eta)+i(2\cos\xi\sin\frac{1}{3}\eta-\sin\frac{2}{3}\eta)]$
$(z/xy)_{12}$	$2\sqrt{3}E_{z,x^2-y^2}(\mathrm{T})\sin\xi\sin\zeta(\cos\frac{1}{3}\eta+i\sin\frac{1}{3}\eta)$
$(z/yz)_{11}$	$E_{z,yz}(0)-2E_{z,yz}(\mathrm{R})(\cos\xi\cos\eta-\cos2\xi)+2\sqrt{3}iE_{z,xz}(\mathrm{R})\cos\xi\sin\eta$
$(z/yz)_{12}$	$-2E_{z,yz}(\mathrm{T})\cos\zeta[(\cos\xi\cos\frac{1}{3}\eta-\cos\frac{2}{3}\eta)+i(\cos\xi\sin\frac{1}{3}\eta+\sin\frac{2}{3}\eta)]$
$(z/xz)_{11}$	$-2\sqrt{3}E_{z,yz}(\mathrm{R})\sin\xi\sin\eta+2iE_{z,xz}(\mathrm{R})(\sin\xi\cos\eta+\sin2\xi)$
$(z/xz)_{12}$	$2\sqrt{3}E_{z,yz}(\mathrm{T})\sin\xi\cos\zeta(\sin\frac{1}{3}\eta-i\cos\frac{1}{3}\eta)$
$(z/x^2-y^2)_{12}$	$2E_{z,x^2-y^2}(\mathrm{T})\sin\zeta[(\cos\xi\sin\frac{1}{3}\eta+\sin\frac{2}{3}\eta)-i(\cos\xi\cos\frac{1}{3}\eta-\cos\frac{2}{3}\eta)]$
$(z/3z^2-r^2)_{12}$	$-2E_{z,3z^2-r^2}(\mathrm{T})\sin\zeta[(2\cos\xi\sin\frac{1}{3}\eta-\sin\frac{2}{3}\eta)-i(2\cos\xi\cos\frac{1}{3}\eta+\cos\frac{2}{3}\eta)]$
$(xy/xy)_{11}$	$E_{xy,xy}(0)+[E_{xy,xy}(\mathrm{R})+3E_{x^2-y^2,x^2-y^2}(\mathrm{R})]\cos\xi\cos\eta+2E_{xy,xy}(\mathrm{R})\cos2\xi$
$(xy/xy)_{12}$	$\cos\zeta\{[E_{xy,xy}(\mathrm{T})+3E_{x^2-y^2,x^2-y^2}(\mathrm{T})]\cos\xi\cos\frac{1}{3}\eta+2E_{xy,xy}(\mathrm{T})\cos\frac{2}{3}\eta\}+i\cos\zeta\{[E_{xy,xy}(\mathrm{T})+3E_{x^2-y^2,x^2-y^2}(\mathrm{T})]\cos\xi\times\sin\frac{1}{3}\eta-2E_{xy,xy}(\mathrm{T})\sin\frac{2}{3}\eta\}$
$(xy/yz)_{12}=(xz/x^2-y^2)_{12}$	$\sqrt{3}[E_{xy,xz}(\mathrm{T})-E_{yz,x^2-y^2}(\mathrm{T})]\sin\xi\sin\zeta(\cos\frac{1}{3}\eta+i\sin\frac{1}{3}\eta)$
$(xy/xz)_{12}$	$\sin\zeta\{-[E_{xy,xz}(\mathrm{T})+3E_{yz,x^2-y^2}(\mathrm{T})]\cos\xi\sin\frac{1}{3}\eta+2E_{xy,xz}(\mathrm{T})\sin\frac{2}{3}\eta\}+i\sin\zeta\{[E_{xy,xz}(\mathrm{T})+3E_{yz,x^2-y^2}(\mathrm{T})]\cos\xi\cos\frac{1}{3}\eta+2E_{xy,xz}(\mathrm{T})\cos\frac{2}{3}\eta\}$

TABLE II.—*Continued.*

$(xy/x^2-y^2)_{11}$	$\sqrt{3}[E_{x^2-y^2,x^2-y^2}(\mathbf{R})-E_{xy,xy}(\mathbf{R})]\sin\xi\sin\eta-2iE_{xy,x^2-y^2}(\mathbf{R})(2\sin\xi\cos\eta-\sin2\xi)$
$(xy/x^2-y^2)_{12}$	$\sqrt{3}[E_{xy,xy}(\mathbf{T})-E_{x^2-y^2,x^2-y^2}(\mathbf{T})]\sin\xi\cos\zeta(\sin\tfrac{1}{3}\eta-i\cos\tfrac{1}{3}\eta)$
$(xy/3z^2-r^2)_{11}$	$-2\sqrt{3}E_{x^2-y^2,3z^2-r^2}(\mathbf{R})\sin\xi\sin\eta+2iE_{xy,3z^2-r^2}(\mathbf{R})(\sin\xi\cos\eta+\sin2\xi)$
$(xy/3z^2-r^2)_{12}$	$2\sqrt{3}E_{x^2-y^2,3z^2-r^2}(\mathbf{T})\sin\xi\cos\zeta(\sin\tfrac{1}{3}\eta-i\cos\tfrac{1}{3}\eta)$
$(yz/yz)_{11}$	$E_{yz,yz}(0)+[E_{yz,yz}(\mathbf{R})+3E_{xz,xz}(\mathbf{R})]\cos\xi\cos\eta+2E_{yz,yz}(\mathbf{R})\cos2\xi$
$(yz/yz)_{12}$	$\cos\zeta\{[E_{yz,yz}(\mathbf{T})+3E_{xz,xz}(\mathbf{T})]\cos\xi\cos\tfrac{1}{3}\eta+2E_{yz,yz}(\mathbf{T})\cos\tfrac{2}{3}\eta\}+i\cos\zeta\{[E_{yz,yz}(\mathbf{T})+3E_{xz,xz}(\mathbf{T})]\cos\xi\sin\tfrac{1}{3}\eta$ $-2E_{yz,yz}(\mathbf{T})\sin\tfrac{2}{3}\eta\}$
$(yz/xz)_{11}$	$\sqrt{3}[E_{yz,yz}(\mathbf{R})-E_{xz,xz}(\mathbf{R})]\sin\xi\sin\eta-2iE_{yz,xz}(\mathbf{R})(2\sin\xi\cos\eta-\sin2\xi)$
$(yz/xz)_{12}$	$\sqrt{3}[E_{xz,xz}(\mathbf{T})-E_{yz,yz}(\mathbf{T})]\sin\xi\cos\zeta(\sin\tfrac{1}{3}\eta-i\cos\tfrac{1}{3}\eta)$
$(yz/x^2-y^2)_{12}$	$\sin\zeta\{-[E_{yz,x^2-y^2}(\mathbf{T})+3E_{xy,xz}(\mathbf{T})]\cos\xi\sin\tfrac{1}{3}\eta+2E_{yz,x^2-y^2}(\mathbf{T})\sin\tfrac{2}{3}\eta\}+i\sin\zeta\{[E_{yz,x^2-y^2}(\mathbf{T})$ $+3E_{xy,xz}(\mathbf{T})]\cos\xi\cos\tfrac{1}{3}\eta+2E_{yz,x^2-y^2}(\mathbf{T})\cos\tfrac{2}{3}\eta\}$
$(yz/3z^2-r^2)_{12}$	$2E_{yz,3z^2-r^2}(\mathbf{T})\sin\zeta[(\cos\xi\sin\tfrac{1}{3}\eta+\sin\tfrac{2}{3}\eta)-i(\cos\xi\cos\tfrac{1}{3}\eta-\cos\tfrac{2}{3}\eta)]$
$(xz/xz)_{11}$	$E_{xz,xz}(0)+[E_{xz,xz}(\mathbf{R})+3E_{yz,yz}(\mathbf{R})]\cos\xi\cos\eta+2E_{xz,xz}(\mathbf{R})\cos2\xi$
$(xz/xz)_{12}$	$\cos\zeta\{[E_{xz,xz}(\mathbf{T})+3E_{yz,yz}(\mathbf{T})]\cos\xi\cos\tfrac{1}{3}\eta+2E_{xz,xz}(\mathbf{T})\cos\tfrac{2}{3}\eta\}+i\cos\zeta\{[E_{xz,xz}(\mathbf{T})+3E_{yz,yz}(\mathbf{T})]\cos\xi\sin\tfrac{1}{3}\eta$ $-2E_{xz,xz}(\mathbf{T})\sin\tfrac{2}{3}\eta\}$
$(xz/3z^2-r^2)_{12}$	$2\sqrt{3}E_{yz,3z^2-r^2}(\mathbf{T})\sin\xi\sin\zeta(\cos\tfrac{1}{3}\eta+i\sin\tfrac{1}{3}\eta)$
$(x^2-y^2/x^2-y^2)_{11}$	$E_{x^2-y^2,x^2-y^2}(0)+[E_{x^2-y^2,x^2-y^2}(\mathbf{R})+3E_{xy,xy}(\mathbf{R})]\cos\xi\cos\eta+2E_{x^2-y^2,x^2-y^2}(\mathbf{R})\cos2\xi$
$(x^2-y^2/x^2-y^2)_{12}$	$\cos\zeta\{[E_{x^2-y^2,x^2-y^2}(\mathbf{T})+3E_{xy,xy}(\mathbf{T})]\cos\xi\cos\tfrac{1}{3}\eta+2E_{x^2-y^2,x^2-y^2}(\mathbf{T})\cos\tfrac{2}{3}\eta\}+i\cos\zeta\{[E_{x^2-y^2,x^2-y^2}(\mathbf{T})+3E_{xy,xy}(\mathbf{T})]$ $\times\cos\xi\sin\tfrac{1}{3}\eta-2E_{x^2-y^2,x^2-y^2}(\mathbf{T})\sin\tfrac{2}{3}\eta\}$
$(x^2-y^2/3z^2-r^2)_{11}$	$E_{x^2-y^2,3z^2-r^2}(0)-2E_{x^2-y^2,3z^2-r^2}(\mathbf{R})(\cos\xi\cos\eta-\cos2\xi)+2\sqrt{3}iE_{xy,3z^2-r^2}(\mathbf{R})\cos\xi\sin\eta$
$(x^2-y^2/3z^2-r^2)_{12}$	$-2E_{x^2-y^2,3z^2-r^2}(\mathbf{T})\cos\zeta[(\cos\xi\cos\tfrac{1}{3}\eta-\cos\tfrac{2}{3}\eta)+i(\cos\xi\sin\tfrac{1}{3}\eta+\sin\tfrac{2}{3}\eta)]$
$(3z^2-r^2/3z^2-r^2)_{11}$	$E_{3z^2-r^2,3z^2-r^2}(0)+2E_{3z^2-r^2,3z^2-r^2}(\mathbf{R})(2\cos\xi\cos\eta+\cos2\xi)$
$(3z^2-r^2/3z^2-r^2)_{12}$	$2E_{3z^2-r^2,3z^2-r^2}(\mathbf{T})\cos\zeta[(2\cos\xi\cos\tfrac{1}{3}\eta+\cos\tfrac{2}{3}\eta)+i(2\cos\xi\sin\tfrac{1}{3}\eta-\sin\tfrac{2}{3}\eta)]$

TABLE III. Matrix components of energy expressed in terms of two-center integrals.

$(s/s)_{11}$	$s_0+2(ss\sigma)_1(2\cos\xi\cos\eta+\cos2\xi)$
$(s/s)_{12}$	$2(ss\sigma)_1\cos\zeta[(2\cos\xi\cos\tfrac{1}{3}\eta+\cos\tfrac{2}{3}\eta)+i(2\cos\xi\sin\tfrac{1}{3}\eta-\sin\tfrac{2}{3}\eta)]$
$(s/x)_{11}$	$2i(sp\sigma)_1(\sin\xi\cos\eta+\sin2\xi)$
$(s/x)_{12}$	$-2(sp\sigma)_1\sin\xi\cos\zeta(\sin\tfrac{1}{3}\eta-i\cos\tfrac{1}{3}\eta)$
$(s/y)_{11}$	$2\sqrt{3}i(sp\sigma)_1\cos\xi\sin\eta$
$(s/y)_{12}$	$\tfrac{2}{3}\sqrt{3}(sp\sigma)_1\cos\zeta[(\cos\xi\cos\tfrac{1}{3}\eta-\cos\tfrac{2}{3}\eta)+i(\cos\xi\sin\tfrac{1}{3}\eta+\sin\tfrac{2}{3}\eta)]$
$(s/z)_{12}$	$-2(\sqrt{\tfrac{2}{3}})(sp\sigma)_1\sin\zeta[(2\cos\xi\sin\tfrac{1}{3}\eta-\sin\tfrac{2}{3}\eta)-i(2\cos\xi\cos\tfrac{1}{3}\eta+\cos\tfrac{2}{3}\eta)]$
$(s/xy)_{11}$	$-3(sd\sigma)_1\sin\xi\sin\eta$
$(s/xy)_{12}$	$-(sd\sigma)_1\sin\xi\cos\zeta(\sin\tfrac{1}{3}\eta-i\cos\tfrac{1}{3}\eta)$
$(s/yz)_{12}$	$-2(\sqrt{\tfrac{2}{3}})(sd\sigma)_1\sin\zeta[(\cos\xi\sin\tfrac{1}{3}\eta+\sin\tfrac{2}{3}\eta)-i(\cos\xi\cos\tfrac{1}{3}\eta-\cos\tfrac{2}{3}\eta)]$
$(s/xz)_{12}$	$-2\sqrt{2}(sd\sigma)_1\sin\xi\sin\zeta(\cos\tfrac{1}{3}\eta+i\sin\tfrac{1}{3}\eta)$
$(s/x^2-y^2)_{11}$	$-\sqrt{3}(sd\sigma)_1(\cos\xi\cos\eta-\cos2\xi)$
$(s/x^2-y^2)_{12}$	$\tfrac{1}{3}\sqrt{3}(sd\sigma)_1\cos\zeta[(\cos\xi\cos\tfrac{1}{3}\eta-\cos\tfrac{2}{3}\eta)+i(\cos\xi\sin\tfrac{1}{3}\eta+\sin\tfrac{2}{3}\eta)]$
$(s/3z^2-r^2)_{11}$	$-(sd\sigma)_1(2\cos\xi\cos\eta+\cos2\xi)$
$(s/3z^2-r^2)_{12}$	$(sd\sigma)_1\cos\zeta[(2\cos\xi\cos\tfrac{1}{3}\eta+\cos\tfrac{2}{3}\eta)+i(2\cos\xi\sin\tfrac{1}{3}\eta-\sin\tfrac{2}{3}\eta)]$
$(x/x)_{11}$	$p_0+[(pp\sigma)_1+3(pp\pi)_1]\cos\xi\cos\eta+2(pp\sigma)_1\cos2\xi$
$(x/x)_{12}$	$\cos\zeta\{[(pp\sigma)_1+3(pp\pi)_1]\cos\xi\cos\tfrac{1}{3}\eta+2(pp\pi)_1\cos\tfrac{2}{3}\eta\}+i\cos\zeta\{[(pp\sigma)_1+3(pp\pi)_1]\cos\xi\sin\tfrac{1}{3}\eta-2(pp\pi)_1\sin\tfrac{2}{3}\eta\}$
$(x/y)_{11}$	$-\sqrt{3}[(pp\sigma)_1-(pp\pi)_1]\sin\xi\sin\eta$
$(x/y)_{12}$	$-\tfrac{1}{3}\sqrt{3}[(pp\sigma)_1-(pp\pi)_1]\sin\xi\cos\zeta(\sin\tfrac{1}{3}\eta-i\cos\tfrac{1}{3}\eta)$
$(x/z)_{12}$	$-2(\sqrt{\tfrac{2}{3}})[(pp\sigma)_1-(pp\pi)_1]\sin\xi\sin\zeta(\cos\tfrac{1}{3}\eta+i\sin\tfrac{1}{3}\eta)$
$(x/xy)_{11}$	$(pd)_0+i[\tfrac{3}{2}(pd\sigma)_1+\sqrt{3}(pd\pi)_1]\cos\xi\sin\eta$
$(x/xy)_{12}$	$\cos\zeta\{[\tfrac{1}{2}(pd\sigma)_1+\tfrac{1}{3}\sqrt{3}(pd\pi)_1]\cos\xi\cos\tfrac{1}{3}\eta-\tfrac{2}{3}\sqrt{3}(pd\pi)_1\cos\tfrac{2}{3}\eta\}+i\cos\zeta\{[\tfrac{1}{2}(pd\sigma)_1+\tfrac{1}{3}\sqrt{3}(pd\pi)_1]\cos\xi\sin\tfrac{1}{3}\eta$ $+\tfrac{2}{3}\sqrt{3}(pd\pi)_1\sin\tfrac{2}{3}\eta\}$
$(x/yz)_{12}=(y/xz)_{12}=(z/xy)_{12}$	$-[(\sqrt{\tfrac{2}{3}})(pd\sigma)_1-\tfrac{2}{3}\sqrt{2}(pd\pi)_1]\sin\xi\sin\zeta(\cos\tfrac{1}{3}\eta+i\sin\tfrac{1}{3}\eta)$
$(x/xz)_{12}$	$\sin\zeta\{-[\sqrt{2}(pd\sigma)_1+2(\sqrt{\tfrac{2}{3}})(pd\pi)_1]\cos\xi\sin\tfrac{1}{3}\eta+2(\sqrt{\tfrac{2}{3}})(pd\pi)_1\sin\tfrac{2}{3}\eta\}+i\sin\zeta\{[\sqrt{2}(pd\sigma)_1+2(\sqrt{\tfrac{2}{3}})(pd\pi)_1]\cos\xi$ $\times\cos\tfrac{1}{3}\eta+2(\sqrt{\tfrac{2}{3}})(pd\pi)_1\cos\tfrac{2}{3}\eta\}$
$(x/x^2-y^2)_{11}$	$i\{-[\tfrac{1}{2}\sqrt{3}(pd\sigma)_1-3(pd\pi)_1]\sin\xi\cos\eta+\sqrt{3}(pd\sigma)_1\sin2\xi\}$
$(x/x^2-y^2)_{12}=(y/xy)_{12}$	$-\tfrac{1}{3}[\tfrac{1}{2}\sqrt{3}(pd\sigma)_1+5(pd\pi)_1]\sin\xi\cos\zeta(\sin\tfrac{1}{3}\eta-i\cos\tfrac{1}{3}\eta)$
$(x/3z^2-r^2)_{11}$	$-i(pd\sigma)_1(\sin\xi\cos\eta+\sin2\xi)$
$(x/3z^2-r^2)_{12}$	$-[(pd\sigma)_1-\tfrac{4}{3}\sqrt{3}(pd\pi)_1]\sin\xi\cos\zeta(\sin\tfrac{1}{3}\eta-i\cos\tfrac{1}{3}\eta)$
$(y/y)_{11}$	$p_0+[3(pp\sigma)_1+(pp\pi)_1]\cos\xi\cos\eta+2(pp\pi)_1\cos2\xi$
$(y/y)_{12}$	$\tfrac{1}{3}\cos\zeta\{[(pp\sigma)_1+11(pp\pi)_1]\cos\xi\cos\tfrac{1}{3}\eta+2[(pp\sigma)_1+2(pp\pi)_1]\cos\tfrac{2}{3}\eta\}+\tfrac{1}{3}i\cos\zeta\{[(pp\sigma)_1+11(pp\pi)_1]\cos\xi\sin\tfrac{1}{3}\eta$ $-2[(pp\sigma)_1+2(pp\pi)_1]\sin\tfrac{2}{3}\eta\}$

TABLE III.—*Continued.*

$(y/z)_{12}$	$-\frac{2}{3}\sqrt{2}[(pp\sigma)_1-(pp\pi)_1]\sin\zeta[(\cos\xi\sin\frac{1}{3}\eta+\sin\frac{2}{3}\eta)-i(\cos\xi\cos\frac{1}{3}\eta-\cos\frac{2}{3}\eta)]$
$(y/xy)_{11}$	$i\{[\frac{3}{2}\sqrt{3}(pd\sigma)_1-(pd\pi)_1]\sin\xi\cos\eta+2(pd\pi)_1\sin2\xi\}$
$(y/yz)_{12}$	$\frac{1}{3}\sin\zeta\{-[\sqrt{2}(pd\sigma)_1+10(\sqrt{\frac{2}{3}})(pd\pi)_1]\cos\xi\sin\frac{1}{3}\eta+2[\sqrt{2}(pd\sigma)_1+(\sqrt{\frac{2}{3}})(pd\pi)_1]\sin\frac{2}{3}\eta\}+\frac{1}{3}i\sin\zeta\{[\sqrt{2}(pd\sigma)_1+10(\sqrt{\frac{2}{3}})(pd\pi)_1]\cos\xi\cos\frac{1}{3}\eta+2[\sqrt{2}(pd\sigma)_1+(\sqrt{\frac{2}{3}})(pd\pi)_1]\cos\frac{2}{3}\eta\}$
$(y/x^2-y^2)_{11}$	$(pd)_0-i[\frac{3}{2}(pd\sigma)_1+\sqrt{3}(pd\pi)_1]\cos\xi\sin\eta$
$(y/x^2-y^2)_{12}$	$\frac{1}{3}\cos\zeta\{[\frac{1}{2}(pd\sigma)_1-(7/3)\sqrt{3}(pd\pi)_1]\cos\xi\cos\frac{1}{3}\eta+2[\frac{1}{2}(pd\sigma)_1+\frac{2}{3}\sqrt{3}(pd\pi)_1]\cos\frac{2}{3}\eta\}+\frac{1}{3}i\cos\zeta\{[\frac{1}{2}(pd\sigma)_1-(7/3)\sqrt{3}(pd\pi)_1]\cos\xi\sin\frac{1}{3}\eta-2[\frac{1}{2}(pd\sigma)_1+\frac{2}{3}\sqrt{3}(pd\pi)_1]\sin\frac{2}{3}\eta\}$
$(y/3z^2-r^2)_{11}$	$-\sqrt{3}i(pd\sigma)_1\cos\xi\sin\eta$
$(y/3z^2-r^2)_{12}$	$\frac{1}{3}[\sqrt{3}(pd\sigma)_1-4(pd\pi)_1]\cos\zeta[(\cos\xi\cos\frac{1}{3}\eta-\cos\frac{2}{3}\eta)+i(\cos\xi\sin\frac{1}{3}\eta+\sin\frac{2}{3}\eta)]$
$(z/z)_{11}$	$p_0+2(pp\pi)_1(2\cos\xi\cos\eta+\cos2\xi)$
$(z/z)_{12}$	$\frac{2}{3}[2(pp\sigma)_1+(pp\pi)_1]\cos\zeta[(2\cos\xi\cos\frac{1}{3}\eta+\cos\frac{2}{3}\eta)+i(2\cos\xi\sin\frac{1}{3}\eta-\sin\frac{2}{3}\eta)]$
$(z/yz)_{11}$	$2\sqrt{3}i(pd\pi)_1\cos\xi\sin\eta$
$(z/yz)_{12}$	$\frac{2}{3}[2(pd\sigma)_1-\frac{1}{3}\sqrt{3}(pd\pi)_1]\cos\zeta[(\cos\xi\cos\frac{1}{3}\eta-\cos\frac{2}{3}\eta)+i(\cos\xi\sin\frac{1}{3}\eta+\sin\frac{2}{3}\eta)]$
$(z/xz)_{11}$	$2i(pd\pi)_1(\sin\xi\cos\eta+\sin2\xi)$
$(z/xz)_{12}$	$-\frac{2}{3}[2\sqrt{3}(pd\sigma)_1-(pd\pi)_1]\sin\xi\cos\zeta(\sin\frac{1}{3}\eta-i\cos\frac{1}{3}\eta)$
$(z/x^2-y^2)_{12}$	$-\frac{1}{3}[\sqrt{2}(pd\sigma)_1-2(\sqrt{\frac{2}{3}})(pd\pi)_1]\sin\zeta[(\cos\xi\sin\frac{1}{3}\eta+\sin\frac{2}{3}\eta)-i(\cos\xi\cos\frac{1}{3}\eta-\cos\frac{2}{3}\eta)]$
$(z/3z^2-r^2)_{12}$	$-[(\sqrt{\frac{2}{3}})(pd\sigma)_1+\frac{2}{3}\sqrt{2}(pd\pi)_1]\sin\zeta[(2\cos\xi\sin\frac{1}{3}\eta-\sin\frac{2}{3}\eta)-i(2\cos\xi\cos\frac{1}{3}\eta+\cos\frac{2}{3}\eta)]$
$(xy/xy)_{11}$	$d_0+[(9/4)(dd\sigma)_1+(dd\pi)_1+\frac{3}{4}(dd\delta)_1]\cos\xi\cos\eta+2(dd\pi)_1\cos2\xi$
$(xy/xy)_{12}$	$\cos\zeta\{\frac{1}{4}[(dd\sigma)_1+4(dd\pi)_1+11(dd\delta)_1]\cos\xi\cos\frac{1}{3}\eta+\frac{2}{3}[(dd\pi)_1+2(dd\delta)_1]\cos\frac{2}{3}\eta\}+i\cos\zeta\{\frac{1}{4}[(dd\sigma)_1+4(dd\pi)_1+11(dd\delta)_1]\cos\xi\sin\frac{1}{3}\eta-\frac{2}{3}[(dd\pi)_1+2(dd\delta)_1]\sin\frac{2}{3}\eta\}$
$(xy/yz)_{12}=(xz/x^2-y^2)_{12}$	$-(\sqrt{\frac{2}{3}})[\frac{1}{2}(dd\sigma)_1+\frac{4}{3}(dd\pi)_1-(11/6)(dd\delta)_1]\sin\xi\sin\zeta(\cos\frac{1}{3}\eta+i\sin\frac{1}{3}\eta)$
$(xy/xz)_{12}$	$-\sqrt{2}\sin\zeta\{\frac{1}{2}[(dd\sigma)_1-(dd\delta)_1]\cos\xi\sin\frac{1}{3}\eta+\frac{2}{3}[(dd\pi)_1-(dd\delta)_1]\sin\frac{2}{3}\eta\}+\sqrt{2}i\sin\zeta\{\frac{1}{2}[(dd\sigma)_1-(dd\delta)_1]\cos\xi\cos\frac{1}{3}\eta-\frac{2}{3}[(dd\pi)_1-(dd\delta)_1]\cos\frac{2}{3}\eta\}$
$(xy/x^2-y^2)_{11}$	$\frac{1}{4}\sqrt{3}[3(dd\sigma)_1-4(dd\pi)_1+(dd\delta)_1]\sin\xi\sin\eta$
$(xy/x^2-y^2)_{12}$	$-\frac{1}{3}\sqrt{3}[\frac{1}{4}(dd\sigma)_1-\frac{1}{3}(dd\pi)_1+(1/12)(dd\delta)_1]\sin\xi\cos\zeta(\sin\frac{1}{3}\eta-i\cos\frac{1}{3}\eta)$
$(xy/3z^2-r^2)_{11}$	$\frac{3}{2}[(dd\sigma)_1-(dd\delta)_1]\sin\xi\sin\eta$
$(xy/3z^2-r^2)_{12}$	$-[\frac{1}{2}(dd\sigma)_1-\frac{4}{3}(dd\pi)_1+\frac{5}{6}(dd\delta)_1]\sin\xi\cos\zeta(\sin\frac{1}{3}\eta-i\cos\frac{1}{3}\eta)$
$(yz/yz)_{11}$	$d_1+[3(dd\pi)_1+(dd\delta)_1]\cos\xi\cos\eta+2(dd\delta)_1\cos2\xi$
$(yz/yz)_{12}$	$\frac{1}{3}\cos\zeta\{[2(dd\sigma)_1+(19/3)(dd\pi)_1+(11/3)(dd\delta)_1]\cos\xi\cos\frac{1}{3}\eta+2[2(dd\sigma)_1+\frac{1}{3}(dd\pi)_1+\frac{2}{3}(dd\delta)_1]\cos\frac{2}{3}\eta\}+\frac{1}{3}i\cos\zeta\{[2(dd\sigma)_1+(19/3)(dd\pi)_1+(11/3)(dd\delta)_1]\cos\xi\sin\frac{1}{3}\eta-2[2(dd\sigma)_1+\frac{1}{3}(dd\pi)_1+\frac{2}{3}(dd\delta)_1]\sin\frac{2}{3}\eta\}$
$(yz/xz)_{11}$	$-\sqrt{3}[(dd\pi)_1-(dd\delta)_1]\sin\xi\sin\eta$
$(yz/xz)_{12}$	$-\frac{1}{3}\sqrt{3}[2(dd\sigma)_1-(5/3)(dd\pi)_1-\frac{1}{3}(dd\delta)_1]\sin\xi\cos\zeta(\sin\frac{1}{3}\eta-i\cos\frac{1}{3}\eta)$
$(yz/x^2-y^2)_{12}$	$-\frac{1}{3}\sqrt{2}\sin\zeta\{[\frac{1}{2}(dd\sigma)_1-(8/3)(dd\pi)_1+(13/6)(dd\delta)_1]\cos\xi\sin\frac{1}{3}\eta-[(dd\sigma)_1+\frac{2}{3}(dd\pi)_1-(5/3)(dd\delta)_1]\sin\frac{2}{3}\eta\}+\frac{1}{3}\sqrt{2}i\sin\zeta\{[\frac{1}{2}(dd\sigma)_1-(8/3)(dd\pi)_1+(13/6)(dd\delta)_1]\cos\xi\cos\frac{1}{3}\eta+[(dd\sigma)_1+\frac{2}{3}(dd\pi)_1-(5/3)(dd\delta)_1]\cos\frac{2}{3}\eta\}$
$(yz/3z^2-r^2)_{12}$	$-2(\sqrt{\frac{2}{3}})[\frac{1}{2}(dd\sigma)_1-\frac{1}{3}(dd\pi)_1-\frac{1}{6}(dd\delta)_1]\sin\zeta[(\cos\xi\sin\frac{1}{3}\eta+\sin\frac{2}{3}\eta)-i(\cos\xi\cos\frac{1}{3}\eta-\cos\frac{2}{3}\eta)]$
$(xz/xz)_{11}$	$d_1+[(dd\pi)_1+3(dd\delta)_1]\cos\xi\cos\eta+2(dd\pi)_1\cos2\xi$
$(xz/xz)_{12}$	$\cos\zeta\{[2(dd\sigma)_1+(dd\pi)_1+(dd\delta)_1]\cos\xi\cos\frac{1}{3}\eta+\frac{2}{3}[2(dd\pi)_1+(dd\delta)_1]\cos\frac{2}{3}\eta\}+i\cos\zeta\{[2(dd\sigma)_1+(dd\pi)_1+(dd\delta)_1]\times\cos\xi\sin\frac{1}{3}\eta-\frac{2}{3}[2(dd\pi)_1+(dd\delta)_1]\sin\frac{2}{3}\eta\}$
$(xz/3z^2-r^2)_{12}$	$-2\sqrt{2}[\frac{1}{2}(dd\sigma)_1-\frac{1}{3}(dd\pi)_1-\frac{1}{6}(dd\delta)_1]\sin\xi\sin\zeta(\cos\frac{1}{3}\eta+i\sin\frac{1}{3}\eta)$
$(x^2-y^2/x^2-y^2)_{11}$	$d_0+[\frac{3}{4}(dd\sigma)_1+3(dd\pi)_1+\frac{1}{4}(dd\delta)_1]\cos\xi\cos\eta+\frac{1}{2}[3(dd\sigma)_1+(dd\delta)_1]\cos2\xi$
$(x^2-y^2/x^2-y^2)_{12}$	$\frac{1}{3}\cos\zeta\{[\frac{1}{4}(dd\sigma)_1+(11/3)(dd\pi)_1+(97/12)(dd\delta)_1]\cos\xi\cos\frac{1}{3}\eta+2[\frac{1}{4}(dd\sigma)_1+\frac{2}{3}(dd\pi)_1+(25/12)(dd\delta)_1]\cos\frac{2}{3}\eta\}+\frac{1}{3}i\cos\zeta\{[\frac{1}{4}(dd\sigma)_1+(11/3)(dd\pi)_1+(97/12)(dd\delta)_1]\cos\xi\sin\frac{1}{3}\eta-2[\frac{1}{4}(dd\sigma)_1+\frac{2}{3}(dd\pi)_1+(25/12)(dd\delta)_1]\times\sin\frac{2}{3}\eta\}$
$(x^2-y^2/3z^2-r^2)_{11}$	$\frac{1}{2}\sqrt{3}[(dd\sigma)_1-(dd\delta)_1](\cos\xi\cos\eta-\cos2\xi)$
$(x^2-y^2/3z^2-r^2)_{12}$	$\frac{2}{3}\sqrt{3}[\frac{1}{4}(dd\sigma)_1-\frac{2}{3}(dd\pi)_1+(5/12)(dd\delta)_1]\cos\zeta[(\cos\xi\cos\frac{1}{3}\eta-\cos\frac{2}{3}\eta)+i(\cos\xi\sin\frac{1}{3}\eta+\sin\frac{2}{3}\eta)]$
$(3z^2-r^2/3z^2-r^2)_{11}$	$d_2+\frac{1}{2}[(dd\sigma)_1+3(dd\delta)_1](2\cos\xi\cos\eta+\cos2\xi)$
$(3z^2-r^2/3z^2-r^2)_{12}$	$[\frac{1}{2}(dd\sigma)_1+\frac{4}{3}(dd\pi)_1+\frac{1}{6}(dd\delta)_1]\cos\zeta[(2\cos\xi\cos\frac{1}{3}\eta+\cos\frac{2}{3}\eta)+i(2\cos\xi\sin\frac{1}{3}\eta-\sin\frac{2}{3}\eta)]$

volving $\mathbf{r}_i=\mathbf{R}=(2,0,0)$ and nonvanishing E integrals in $(m/n)_{12}$ can be expressed in terms of E integrals involving $\mathbf{r}_i+\mathbf{t}_2=\mathbf{T}=(0,-\frac{2}{3},1)$. We have, for instance

$$E_{y,xy}(1,-1,0)=\tfrac{3}{4}E_{x,x^2-y^2}(\mathbf{R})-\tfrac{1}{4}\sqrt{3}E_{x,xy}(\mathbf{R})+\tfrac{1}{4}\sqrt{3}E_{y,x^2-y^2}(\mathbf{R})-\tfrac{1}{4}E_{x,xy}(\mathbf{R}).$$

After all these reductions, it turns out that only 71 independent E integrals remain. The matrix components of energy expressed in terms of E integrals are given in Table II. In this table we have used the abbreviations $\xi=\frac{1}{2}ak_x$, $\eta=\frac{1}{2}\sqrt{3}ak_y$, $\zeta=\frac{1}{2}ck_z=(\sqrt{\frac{2}{3}})ak_z$.

We make finally the two-center approximation. Here Table I of reference 1 has been used. Upon making this approximation, we have only 16 independent integrals. The nonvanishing matrix components expressed in terms of them are given in Table III.

The author wishes to thank Dr. M. Suffczynski for suggesting the present work and for his continued interest in it.