be expanded in the same way. In the integral (2), we shall get a nonvanishing contribution only if we are dealing with σ components of both ψ_n and ψ_m, or π_+ components of both, or π_- components of both, etc. Hence we can reduce all the various integrals appearing in (2) to a relatively small number.

It is a straightforward matter of rotating axes and transforming spherical harmonics in terms of one set of axes into spherical harmonics with respect to another set, to find the nature of these integrals. Thus, let the atomic orbitals be set up with respect to a set of rectangular axes. We shall symbolize the p_x, p_y, p_z functions by x, y, z; the various d functions by xy, yz, zx, x^2-y^2, and $3z^2-r^2$, which stand for the various functions whose dependence on angle is like that of the polynomials we have written, multiplied by appropriate functions of r. Then to set up the integrals in (2), we need contributions consisting of a product of an atomic orbital of this type on the atom located at $\mathbf{R}_i$, another atomic orbital on the atom at $\mathbf{R}_j$, and spherical potentials centered on these two atoms. Let the direction cosines of the direction of the vector $\mathbf{R}_j-\mathbf{R}_i$, pointing from one atom to the other, be l, m, n. Then we can symbolize one of the integrals by such a symbol as $E_{x,\,xy}(l,m,n)$, meaning an integral in which the function ψ_n is a p_x-like function; ψ_m, a d function with symmetry properties like xy. This particular function can be written approximately in terms of two integrals: that between a $p\sigma$ orbital on the first atom and a $d\sigma$ orbital on the second; and that between a $p\pi$ on the first and a $d\pi$ on the second. Let the first of these be symbolized by $(pd\sigma)$ and the second by $(pd\pi)$; we shall assume that the first index, such as p, refers to the first orbital, the second, as d, to the second, and note that interchanging the order of the indices has no effect if the sum of the parities of the two orbitals is even, but changes the sign if the sum of the parities is odd. We now find, by carrying out the analysis mentioned earlier, that $E_{x,\,xy}(l,m,n)=\sqrt{3}l^2m(pd\sigma)+m(1-2l^2)(pd\pi)$. Similar formulas can be worked out for each of the combinations of functions, and are listed in Table I for all combinations of s, p, and d functions. The entries not given in the table can be found by cyclically permuting the coordinates and direction cosines. It is to be realized, of course, that the integrals like $(pd\sigma)$ are functions of the distance between the atoms, so

TABLE I. Energy integrals for crystal in terms of two-center integrals.

$E_{s,\,s}$	$(ss\sigma)$
$E_{s,\,x}$	$l(sp\sigma)$
$E_{x,\,x}$	$l^2(pp\sigma)+(1-l^2)(pp\pi)$
$E_{x,\,y}$	$lm(pp\sigma)-lm(pp\pi)$
$E_{x,\,z}$	$ln(pp\sigma)-ln(pp\pi)$
$E_{s,\,xy}$	$\sqrt{3}lm(sd\sigma)$
$E_{s,\,x^2-y^2}$	$\frac{1}{2}\sqrt{3}(l^2-m^2)(sd\sigma)$
$E_{s,\,3z^2-r^2}$	$[n^2-\frac{1}{2}(l^2+m^2)](sd\sigma)$
$E_{x,\,xy}$	$\sqrt{3}l^2m(pd\sigma)+m(1-2l^2)(pd\pi)$
$E_{x,\,yz}$	$\sqrt{3}lmn(pd\sigma)-2lmn(pd\pi)$
$E_{x,\,zx}$	$\sqrt{3}l^2n(pd\sigma)+n(1-2l^2)(pd\pi)$
$E_{x,\,x^2-y^2}$	$\frac{1}{2}\sqrt{3}l(l^2-m^2)(pd\sigma)+l(1-l^2+m^2)(pd\pi)$
$E_{y,\,x^2-y^2}$	$\frac{1}{2}\sqrt{3}m(l^2-m^2)(pd\sigma)-m(1+l^2-m^2)(pd\pi)$
$E_{z,\,x^2-y^2}$	$\frac{1}{2}\sqrt{3}n(l^2-m^2)(pd\sigma)-n(l^2-m^2)(pd\pi)$
$E_{x,\,3z^2-r^2}$	$l[n^2-\frac{1}{2}(l^2+m^2)](pd\sigma)-\sqrt{3}ln^2(pd\pi)$
$E_{y,\,3z^2-r^2}$	$m[n^2-\frac{1}{2}(l^2+m^2)](pd\sigma)-\sqrt{3}mn^2(pd\pi)$
$E_{z,\,3z^2-r^2}$	$n[n^2-\frac{1}{2}(l^2+m^2)](pd\sigma)+\sqrt{3}n(l^2+m^2)(pd\pi)$
$E_{xy,\,xy}$	$3l^2m^2(dd\sigma)+(l^2+m^2-4l^2m^2)(dd\pi)+(n^2+l^2m^2)(dd\delta)$
$E_{xy,\,yz}$	$3lm^2n(dd\sigma)+ln(1-4m^2)(dd\pi)+ln(m^2-1)(dd\delta)$
$E_{xy,\,zx}$	$3l^2mn(dd\sigma)+mn(1-4l^2)(dd\pi)+mn(l^2-1)(dd\delta)$
$E_{xy,\,x^2-y^2}$	$\frac{3}{2}lm(l^2-m^2)(dd\sigma)+2lm(m^2-l^2)(dd\pi)+\frac{1}{2}lm(l^2-m^2)(dd\delta)$
$E_{yz,\,x^2-y^2}$	$\frac{3}{2}mn(l^2-m^2)(dd\sigma)-mn[1+2(l^2-m^2)](dd\pi)+mn[1+\frac{1}{2}(l^2-m^2)](dd\delta)$
$E_{zx,\,x^2-y^2}$	$\frac{3}{2}nl(l^2-m^2)(dd\sigma)+nl[1-2(l^2-m^2)](dd\pi)-nl[1-\frac{1}{2}(l^2-m^2)](dd\delta)$
$E_{xy,\,3z^2-r^2}$	$\sqrt{3}lm[n^2-\frac{1}{2}(l^2+m^2)](dd\sigma)-2\sqrt{3}lmn^2(dd\pi)+\frac{1}{2}\sqrt{3}lm(1+n^2)(dd\delta)$
$E_{yz,\,3z^2-r^2}$	$\sqrt{3}mn[n^2-\frac{1}{2}(l^2+m^2)](dd\sigma)+\sqrt{3}mn(l^2+m^2-n^2)(dd\pi)-\frac{1}{2}\sqrt{3}mn(l^2+m^2)(dd\delta)$
$E_{zx,\,3z^2-r^2}$	$\sqrt{3}ln[n^2-\frac{1}{2}(l^2+m^2)](dd\sigma)+\sqrt{3}ln(l^2+m^2-n^2)(dd\pi)-\frac{1}{2}\sqrt{3}ln(l^2+m^2)(dd\delta)$
$E_{x^2-y^2,\,x^2-y^2}$	$\frac{3}{4}(l^2-m^2)^2(dd\sigma)+[l^2+m^2-(l^2-m^2)^2](dd\pi)+[n^2+\frac{1}{4}(l^2-m^2)^2](dd\delta)$
$E_{x^2-y^2,\,3z^2-r^2}$	$\frac{1}{2}\sqrt{3}(l^2-m^2)[n^2-\frac{1}{2}(l^2+m^2)](dd\sigma)+\sqrt{3}n^2(m^2-l^2)(dd\pi)+\frac{1}{4}\sqrt{3}(1+n^2)(l^2-m^2)(dd\delta)$
$E_{3z^2-r^2,\,3z^2-r^2}$	$[n^2-\frac{1}{2}(l^2+m^2)]^2(dd\sigma)+3n^2(l^2+m^2)(dd\pi)+\frac{3}{4}(l^2+m^2)^2(dd\delta)$