APPENDIX A. SOLID HARMONICS AND MULTIPOLAR EXPANSION OF COULOMB INTERACTION

With reference to a given point C = (C_x, C_y, C_z), and for integer ℓ and m values ($\ell \geq 0$, $|m| \leq \ell$), unnormalized complex solid harmonics are defined as:

$$Y_\ell^m(C;r) = r_C^\ell \, P_\ell^{|m|}(\cos\theta) \, \exp(im\phi) \qquad A.1$$

where r_C, ϕ and θ are the spherical polar coordinates (principal axis z) of the vector:

$$r_C = r - C = (x_C, y_C, z_C) \qquad A.2$$

and $P_\ell^{|m|}$ are the associated Legendre functions.
We also introduce unnormalized real solid harmonics

$$X_\ell^{|m|}(C;r) = \mathrm{Re}\,[Y_\ell^{|m|}(C;r)]$$
$$X_\ell^{-|m|}(C;r) = \mathrm{Im}\,[Y_\ell^{|m|}(C;r)] \qquad A.3$$

After introducing, for integer m, the notation $E(\phi,m)$ to indicate $\cos(|m|\phi)$ for $m \geq 0$ and $\sin(|m|\phi)$ for $m < 0$, equations A.3 can be reformulated as follows:

$$X_\ell^m(C;r) = r_C^\ell \, P_\ell^{|m|}(\cos\theta) \, E(\phi,m) \qquad A.4$$

Real solid harmonics are homogeneous polynomials of degree ℓ in x, y, z:

$$X_\ell^m(C;r) = \sum_{tuv}^{(t+u+v=\ell)} D_\ell^m(t,u,v) \, x_C^t \, y_C^u \, z_C^v \qquad A.5$$

The D coefficients are easily generated using the recursion relations:

$$X_{\ell+1}^{\pm(\ell+1)} = (2\ell+1)\,[x_C \, X_\ell^{\pm\ell} \mp y_C \, X_\ell^{\mp\ell}] \qquad A.6$$

$$X_{\ell+1}^m = [(2\ell+1) \, z_C \, X_\ell^m - (\ell + |m|) \, r_C^2 \, X_{\ell-1}^m] \,/\, (\ell - |m| + 1) \qquad A.7$$

These recursion relations are applied starting from $X_0^0 = 1$ and formally setting $X_0^{-0} = 0$; in the rhs of the above equation $X_\ell^m = 0$ if $|m| > \ell$. A list of the D coefficients up to $\ell = 4$ is provided in Table A.1 below.

Table A.1. Non zero $D_\ell^m(tuv)$ coefficients in the polynomial representation of the real solid harmonics (equation A.5), up to ℓ=4. The triplet of integers in brackets after each coefficient specifies the corresponding exponents t,u,v. For instance:

$X_3^{-3} = 45\ x^2y - 15\ y^3$

(ℓ,m)	Non zero D_ℓ^m(t,u,v)			
(0,0)	1 (0,0,0)			
(1,1)	1 (1,0,0)			
(1,0)	1 (0,0,1)			
(1,-1)	1 (0,1,0)			
(2,2)	3 (2,0,0)	-3 (0,2,0)		
(2,1)	3 (1,0,1)			
(2,0)	-1/2 (2,0,0)	-1/2 (0,2,0)	1 (0,0,2)	
(2,-1)	3 (0,1,1)			
(2,-2)	6 (1,1,0)			
(3,3)	15 (3,0,0)	-45 (1,2,0)		
(3,2)	15 (2,0,1)	-15 (0,2,1)		
(3,1)	-3/2 (3,0,0)	-3/2 (1,2,0)	6 (1,0,2)	
(3,0)	-3/2 (2,0,1)	-3/2 (0,2,1)	1 (0,0,3)	
(3,-1)	-3/2 (2,1,0)	-3/2 (0,3,0)	6 (0,1,2)	
(3,-2)	30 (1,1,1)			
(3,-3)	45 (2,1,0)	-15 (0,3,0)		
(4,4)	105 (4,0,0)	-630 (2,2,0)	105 (0,4,0)	
(4,3)	105 (3,0,1)	-315 (1,2,1)		
(4,2)	-15/2 (4,0,0)	45 (2,0,2)	15/2 (0,4,0)	-45 (0,2,2)
(4,1)	-15/2 (3,0,1)	-15/2 (1,2,1)	10 (1,0,3)	
(4,0)	3/8 (4,0,0)	3/4 (2,2,0)	-3 (2,0,2)	3/8 (0,4,0)
	-3 (0,2,2)	1 (0,0,4)		
(4,-1)	-15/2 (2,1,1)	-15/2 (0,3,1)	10 (0,1,3)	
(4,-2)	-15 (3,1,0)	-15 (1,3,0)	90 (1,1,2)	
(4,-3)	315 (2,1,1)	-105 (0,3,1)		
(4,-4)	420 (3,1,0)	-420 (1,3,0)		

The reciprocal of the distance $|r_1-r|$ between two points can be expressed by the well known Neumann-Laplace expansion . Let (r,θ,ϕ) and (r_1,θ_1,ϕ_1) be the spherical coordinates of r and r_1 with respect to a common reference system with origin at C and let $r_<$ be the smaller and $r_>$ be the larger between r and r_1. Then:

$$|r_1-r|^{-1} = \Sigma_{\ell m}\ \{(\ell-|m|)!\ /\ (\ell+|m|)!\}\ P_\ell^{|m|}(\cos\theta_1)\ P_\ell^{|m|}(\cos\theta)\ \cdot$$

$$\exp\ [im\ (\phi_1-\phi)]\ r_<^\ell\ /\ r_>^{\ell+1} =$$

$$= \Sigma_{\ell m} A_\ell^m P_\ell^{|m|} (\cos\theta_1) P_\ell^{|m|} (\cos\theta) E(\Phi_1,m) E(\Phi,m) r_<^\ell / r_>^{\ell+1} \qquad A.8$$

where $\Sigma_{\ell m}$ means $\sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell}$ and

$$A_\ell^m = (2-\varepsilon_{mo}) (\ell-|m|)! / (\ell+|m|)! \qquad A.9$$

Consider now a charge distribution $\rho(r)$ which is entirely contained in a sphere of radius R centered at C. The potential created by $\rho(r)$ at a point r_1 external to the sphere can be expressed by using the expansion A.8 with $r_< = r$, and $r_> = r_1$:

$$V(r_1) = \int \rho(r)/|r-r_1| \, dr = \Sigma_{\ell m}([(A_\ell^m)^{1/2} \int P_\ell^{|m|}(\cos\theta) E(\Phi,m) r^\ell \rho(r) \, dr] \cdot$$

$$\cdot [(A_\ell^m)^{1/2} P_\ell^{|m|} (\cos\theta_1) E(\Phi_1,m) r_1^{-\ell-1}]) =$$

$$= \Sigma_{\ell m} \gamma_\ell^m(C;\{\rho\}) \Phi_\ell^m(C;r_1) \qquad A.10$$

In equation A.10 the symbols γ and Φ for the multipoles of the distribution ρ and for the field terms have been introduced:

$$\gamma_\ell^m (C;\{\rho\}) = (A_\ell^m)^{1/2} \int X_\ell^m (C;r) \rho(r) \, dr \qquad A.11$$

$$\Phi_\ell^m(C;r) = (A_\ell^m)^{1/2} X_\ell^m(C;r) r_C^{-2\ell-1} \qquad A.12$$

(Note that the partition of the A factor between the multipole and the field term is a matter of convention). Owing to equation A.10, we can interpret the general field term $\Phi_\ell^m(C;r)$ as the potential created at r by a point charge distribution centered at C which has all multipoles equal to zero except for the one of indices (ℓ,m) which is unity. A possible definition of such a charge distribution has been provided in section II.2, equation II.2.21, which exploits the orthogonality properties of the spherical harmonics. The overall field created by a general point distribution at a point which is external to the distribution in the sense specified above, can then be seen as a superposition of the Φ_ℓ^m fields, with weights $\gamma_\ell^m (C;\{\rho\})$.

A useful relationship exists between the real solid harmonics and the spherical gradient operator W_ℓ^m. The expression for the latter is obtained by simply substituting in equation A.5 x_C by $\partial/\partial x_C$, and similarly for the other coordinates (Hobson 1931):

$$W_\ell^m (C) = \sum_{tuv}^{(t+u+v=\ell)} D_\ell^m (t,u,v) (\partial/\partial x_C)^t (\partial/\partial y_C)^u (\partial/\partial z_C)^v \qquad A.13$$

The following relation can be shown to hold:

$$W_\ell^m (C) r_C^{-1} = [(2\ell-1)!!] X_\ell^m (C;r) r_C^{-2\ell-1} \qquad A.14$$

APPENDIX B. DEFINITION OF BRILLOUIN ZONE AND RELATED QUANTITIES

Consider the abelian group G of the crystal translations, whose general operator T^g effects a translation by a direct lattice vector $\mathbf{g}$. After introducing the periodic Born-von Karman boundary conditions, G becomes a cyclic group which is the direct product of d groups of order M, d being the dimensionality of the crystal, and M an arbitrarily large but fixed integer. The projection operators for the irreducible one-dimensional representations of the group are of the form:

$$P(\mathbf{k}) = N^{-1/2} \Sigma_g \exp(i\, \mathbf{k}\cdot\mathbf{g})\, P^g \qquad \text{B.1}$$

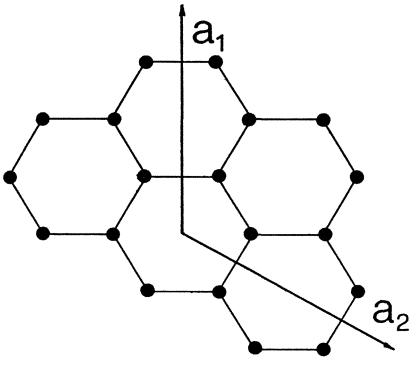
where $N = M^d$ and the general "reciprocal space vector (or point)" $\mathbf{k}$ belongs to a net of vectors, which reproduces the reciprocal lattice shrunk by a factor M. That is, if $\mathbf{B}_i$ are the fundamental reciprocal lattice vectors, related to the direct lattice fundamental vectors $\mathbf{a}_j$ by the relation:

$$\mathbf{B}_i \cdot \mathbf{a}_j = 2\pi\, \delta_{ij} \qquad [\, i = 1,\ldots,d\,]\ , \qquad \text{B.2}$$

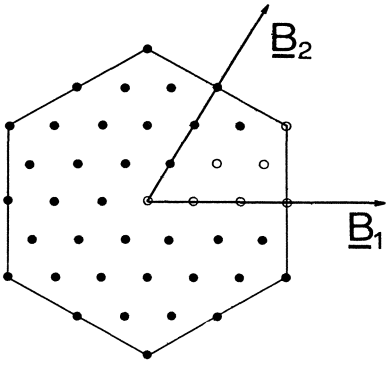
then the $\mathbf{k}$ vectors are of the form:

$$\mathbf{k} = \frac{1}{M} \Sigma_{i=1}^{d}\, n_i\, \mathbf{B}_i \qquad \text{B.3}$$

with integer n_i. It follows from the definition that projection operators are equivalent if they refer to $\mathbf{k}$ vectors that differ by a reciprocal lattice vector $\mathbf{K}$. One may then consider only the $N = M^d$ inequivalent $\mathbf{k}$ points that belong to the first Brillouin Zone (BZ), that is to the Wigner-Seitz cell of reciprocal space. The scheme below illustrates these concepts in the case of graphite, with M = 6. The $\mathbf{k}$ points are indicated with dots.



Direct lattice.



Reciprocal lattice.
The hexagon is the first BZ; open circles represent $\mathbf{k}$ points belonging to IBZ (see below)

By applying the projection operator $P(\mathbf{k})$ to the ω-th AO in the reference zero cell ($\omega = 1,\ldots,p$), a Bloch function (BF) is generated that belongs to the $\mathbf{k}$-th irreducible representation (IR) of G:

$$P(\mathbf{k})\ \chi^{o}_{\omega} = N^{-1/2}\ \Sigma_{g}\ \chi^{g}_{\omega}\ \exp(i\ \mathbf{k}\cdot\mathbf{g}) = \phi_{\omega}(\mathbf{k}) \qquad \text{B.4}$$

The general crystalline orbital (CO) belonging to the $\mathbf{k}$-th IR may be written as (see equation II.3.1):

$$\psi_{j}(\mathbf{k}) = \Sigma^{p}_{\omega=1}\ a_{\omega j}(\mathbf{k})\ \phi_{\omega}(\mathbf{k}) \qquad \text{B.5}$$

Since the $\mathbf{k}$ points are uniformly distributed over the BZ, sums over $\mathbf{k}$ points within a certain portion A of the BZ can be substituted by integrals over A:

$$\Sigma_{\mathbf{k}\epsilon A}\ f(\mathbf{k}) = (N/V_{B})\ \int_{A} d\mathbf{k}\ f(\mathbf{k}) \qquad \text{B.6}$$

where V_B is the volume of the BZ. Suppose now that there are $N = Nq$ electrons in the crystal, that is, q electrons per unit cell. The Fermi energy ϵ_F that identifies the occupied manifold has to be determined by imposing that there are $N/2$ COs whose eigenvalue $\epsilon_j(\mathbf{k})$ is less than ϵ_F. Using the Heaviside step function θ and equation B.6, we can write the following equation that defines implicitly ϵ_F:

$$q = (2/N)\ \Sigma_{j}\ \Sigma_{\mathbf{k}}\ \theta[\epsilon_{F}-\epsilon_{j}(\mathbf{k})] = (2/V_{B})\ \Sigma_{j}\ \int_{BZ} d\mathbf{k}\ \theta[\epsilon_{F}-\epsilon_{j}(\mathbf{k})] \qquad \text{B.7}$$

The following equation is easily seen to hold true:

$$(1/V_{B})\ \int_{BZ} d\mathbf{k}\ \exp(i\ \mathbf{k}\cdot\mathbf{g}) = \delta_{go} \qquad \text{B.8}$$

which is important in the transformation from direct to reciprocal space quantities, and viceversa (see section II.2a).

Exploiting point symmetry makes it possible to consider only crystalline orbitals associated with $\mathbf{k}$ points that belong to the "irreducible part of the BZ" (IBZ). The IBZ is defined so that a general $\mathbf{k}$ point in the BZ is carried onto a $\mathbf{k}$ point in IBZ by a proper or improper rotation V of the point group of the crystal: $\mathbf{k} = V\ \mathbf{k}^{V}$, while no such relation exists between two different points in IBZ. The relation between $\psi_j(\mathbf{k})$ and $\psi_j(\mathbf{k}^V)$, and the corresponding ones for $F(\mathbf{k})$, $S(\mathbf{k})$, $P(\mathbf{k})$, etc are given in section II.7c .

APPENDIX C. THE McMURCHIE-DAVIDSON TECHNIQUE FOR THE EVALUATION OF THE MOLECULAR INTEGRALS

In this appendix we summarize the strategy and the formulae proposed by McMurchie and Davidson (1978) for the evaluation of the mono- and bielectronic integrals, except for field and multipole integrals which are treated in more detail in Section II.4c. The integral package used in CRYSTAL has been derived from the one developed by Saunders (1983) for molecular calculations; here, we use the notation and the sequence of arguments as adopted by that author.

C1. Hermite Gaussian Type Function (HGTF)

Following McMurchie and Davidson (1978) HGTFs are adopted as useful intermediaries for the evaluation of integrals. The HGTFs can be defined through

$$\Lambda[a,\mathbf{A};i,j,k] = \left(\frac{\partial}{\partial A_x}\right)^i \left(\frac{\partial}{\partial A_y}\right)^j \left(\frac{\partial}{\partial A_z}\right)^k \exp(-ar_A^2) \qquad \text{C1.1}$$

where

$$r_A \equiv (x_A,y_A,z_A) = \mathbf{r}-\mathbf{A} = (x-A_x,y-A_y,z-A_z) \qquad \text{C1.2}$$

From equation C1.1 it is obvious that HGTFs are separable in x,y and z functions :

$$\Lambda[a,\mathbf{A};i,j,k] = \Lambda_x[a,\mathbf{A},i]\,\Lambda_y[a,\mathbf{A},j]\,\Lambda_z[a,\mathbf{A},k] \qquad \text{C1.3}$$

$$\Lambda_x[a,\mathbf{A},i] = \left(\frac{\partial}{\partial A_x}\right)^i \exp(-ax_A^2) = \lambda_x[a,\mathbf{A},i]\exp(-ax_A^2) \qquad \text{C1.4}$$

and similarly for Λ_y and Λ_z. In equation C1.4, $\lambda_x[a,\mathbf{A},i]$ is a polynomial of degree i in x, related to the Hermite polynomial H_i as follows:

$$\lambda_x[a,\mathbf{A},i] = a^{i/2} H_i(a^{1/2} x_A) \qquad \text{C1.5}$$

A recursion relation for λ_x can be obtained from the corresponding expression for the Hermite polynomials:

$$x_A\,\lambda_x[a,\mathbf{A},i] = \lambda_x[a,\mathbf{A},i+1]/(2a) + i\,\lambda_x[a,\mathbf{A},i-1] \qquad \text{C1.6}$$

The following useful expressions are easily obtained from equation C1.6 with reference to an origin $C\equiv(C_x,C_y,C_z)$, so that $x_A=x_C-(A_x-C_x)$:

$$x_C\,\lambda_x[A,i] = \lambda_x[A,i+1]/(2a) + (A_x-C_x)\,\lambda_x[A,i] + i\,\lambda_x[A,i-1] \qquad \text{C1.7}$$

$$x_C^2\,\lambda_x[A,i] = \lambda_x[A,i+2]/(2a)^2 + (A_x-C_x)\lambda_x[A,i+1]/a + \{(2i+1)/(2a)+(A_x-C_x)^2\}\cdot$$
$$\cdot\,\lambda_x[A,i] + 2i\,(A_x-C_x)\,\lambda_x[A,i-1] + i(i-1)\,\lambda_x[A,i-2] \qquad \text{C1.8}$$

We have here indicated $\lambda_x[a,\mathbf{A},i]$ by $\lambda_x[A,i]$.
From the properties of the Hermite polynomials it easily follows that the polynomials $\lambda_x[A,i]$ are orthogonal for different i's through the weight function $\exp(-ar_A^2)$. In particular, since $\Lambda[a,\mathbf{A};0,0,0]= \exp(-ar_A^2)$ we have :

$$\int dr\ \Lambda[a,\mathbf{A};i,j,k] = \varsigma_{io}\ \varsigma_{jo}\ \varsigma_{ko}(\pi/a)^{3/2} \qquad \text{C1.9}$$

C2. The Gaussian product theorem and the expansion in HGTF

Let us consider the product of two atomic orbitals located at **A** and **B** (see equations II.2.3-4-5):

$$\chi_\omega(r_A)\ \chi_{\omega'}(r_B) = \sum_{i=1}^{t_{n\ell}} \sum_{j=1}^{t_{n'\ell'}} d_{n\ell,i}^{(\omega)}\ d_{n'\ell',j}^{(\omega')}\ N_\ell^m(a_i)\ N_{\ell'}^{m'}(b_j)\ \cdot$$

$$\cdot\ X_\ell^m(\mathbf{A};r)\ X_{\ell'}^{m'}(\mathbf{B};r)\ \exp(-a_i r_A^2)\ \exp(-b_j r_B^2) \qquad \text{C2.1}$$

Using the Gaussian product theorem (Boys 1950), we can write :

$$\exp(-ar_A^2)\ \exp(-br_B^2) = K_{AB}\ \exp(-pr_P^2) \qquad \text{C2.2}$$

where:

$$p = a+b\ ; \quad \mathbf{P} = (a\mathbf{A}+b\mathbf{B})/(a+b)\ ; \quad K_{AB} = \exp[-ab\ (\mathbf{A}-\mathbf{B})^2/p] \qquad \text{C2.3}$$

Real solid harmonics $X_\ell^m(\mathbf{A};r)$ are polynomials of degree ℓ in x,y and z (see Appendix A). The product $X_\ell^m(\mathbf{A};r)\ X_{\ell'}^{m'}(\mathbf{B};r)$ can then be written as a polynomial of degree $\ell+\ell'$ in x_P, y_P, z_P or, equivalently, as a linear combination of Hermite polynomials of degree t, u, v in x_P, y_P, z_P, with $t+u+v \leq \ell+\ell'$:

$$X_\ell^m(\mathbf{A};r)\ X_{\ell'}^{m'}(\mathbf{B};r) = \Sigma_{tuv}\ E[\ell,m;\ell',m';t,u,v]\ \lambda[p,\mathbf{P};t,u,v] \qquad \text{C2.4}$$

where $\lambda \equiv \lambda_x\ \lambda_y\ \lambda_z$ (see equation C1.4). Note that, because $X_0^0=1$:

$$E[0,0;0,0;0,0,0] = 1 \qquad \text{C2.5}$$

For each couple of primitives one has to generate all the E coefficients such that $t+u+v \leq \ell+\ell'$. We will illustrate in the next section the recursion relations for this purpose. Equation C2.1 then becomes:

$$\chi_\omega(r_A)\ \chi_{\omega'}(r_B) = \sum_{i=1}^{t_{n\ell}} \sum_{j=1}^{t_{n'\ell'}} \Sigma_{tuv}\ F[\omega,i;\omega',j;t,u,v]\ \Lambda[p,\mathbf{P};t,u,v] \qquad \text{C2.6}$$

$$F[\omega,i;\omega',j;t,u,v] =$$

$$= d_{n\ell,i}^{(\omega)}\ d_{n'\ell',j}^{(\omega')}\ N_\ell^m(a_i)\ N_{\ell'}^{m'}(b_j)\ K_{AB}\ E[\ell,m;\ell',m',t,u,v] \qquad \text{C2.7}$$

To simplify the notation, here and in the following we will assume that in equation C2.6 one has $t_{n\ell}=t_{n'\ell'}=1$ (a single gaussian per AO), so that the double summation over i and j reduces to a single term.

C3. The expansion coefficients E

a) Recursion in ℓ

According to equation C2.4 we have :

$$X^{m}_{\ell+1}(A;r)\; X^{m'}_{\ell'}(B;r) = \Sigma_{tuv}\; E[\ell+1;t,u,v]\; \lambda[P;t,u,v] \qquad C3.1$$

where, for compactness, the index p has been omitted from λ, and m,ℓ',m' have been omitted from E.
On the other hand, a combination of equations A7 and C2.4 yields:

$$X^{m}_{\ell+1}(A;r)\; X^{m'}_{\ell'}(B;r) = \Sigma_{tuv}\{\; E[\ell;t,u,v]\; (2\ell+1)\; z_A\; \lambda[P;t,u,v] +$$

$$-\; E[\ell-1;t,u,v]\; (\ell+|m|)\; r_A^2\; \lambda[P;t,u,v]\; \}/(\ell-|m|+1) \qquad C3.2$$

The recursion relations C1.7 and C1.8 can now be used in eq. C3.2 ($r_A^2 = x_A^2 + y_A^2 + z_A^2$); grouping the resulting coefficients of the general $\lambda[t,u,v]$ term, equating with the corresponding term in equation C2.4, and defining $\mathbf{D} \equiv \mathbf{P}-\mathbf{A} \equiv (D_x,D_y,D_z)$ gives:

$$E[\ell+1;t,u,v] =$$

$$= \{E[\ell;t,u,v-1]/(2p)+ D_z\; E(\ell;t,u,v) + (v+1)\; E[\ell;t,u,v+1]\}\cdot$$

$$\cdot[(2\ell+1)/(\ell-|m|+1)] \;-\; [(\ell+|m|)/(\ell-|m|+1)]\cdot$$

$$\cdot\{\; (E[\ell-1;t-2,u,v] + E[\ell-1;t,u-2,v] + E[\ell-1;t,u,v-2])/(2p)^2 +$$

$$+ (D_x\; E[\ell-1;t-1,u,v] + D_y\; E[\ell-1;t,u-1,v] + D_z\; E[\ell-1;t,u,v-1])/p +$$

$$+ (D^2+(2t+2u+2v+3)/(2p))\; E[\ell-1;t,u,v] + 2D_x(t+1)\; E[\ell-1;t+1,u,v] +$$

$$+ 2D_y(u+1)\; E[\ell-1;t,u+1,v] + 2D_z(v+1)\; E[\ell-1;t,u,v+1] +$$

$$+ (t+2)(t+1)\; E[\ell-1;t+2,u,v] + (u+2)(u+1)\; E[\ell-1;t,u+2,v] +$$

$$+ (v+2)(v+1)\; E[\ell-1;t,u,v+2]\; \} \qquad C3.3$$

b) Recursion in ℓ and $|m|=\ell$

Consider first the case $m = \ell$; from equations A.6 and C2.4 we have:

$$X^{\ell+1}_{\ell+1}(A;r)\; X^{m'}_{\ell'}(B;r) = (2\ell+1)\Sigma_{tuv}\{\; E[\ell,\ell;t,u,v]\; x_A\; \lambda[t,u,v] +$$

$$- E[\ell,-\ell;t,u,v]\; y_A\; \lambda[t,u,v]\;\} \qquad \text{C3.4}$$

where the indices ℓ',m' have again been omitted from E, and p,P from λ. Using equation C1.7 and comparing the result with equation C2.4, gives:

$$E[\ell+1,\ell+1;t,u,v] = (2\ell+1)\;\{\; E[\ell,\ell;t-1,u,v]/(2p) - E[\ell,-\ell;t,u-1,v]/(2p) +$$

$$+ D_x\; E[\ell,\ell;t,u,v] - D_y\; E[\ell,-\ell;t,u,v] +$$

$$+ (t+1)E[\ell,\ell;t+1,u,v] - (u+1)E[\ell,-\ell;t,u+1,v]\;\} \qquad \text{C3.5}$$

In a similar way we obtain for $m=-\ell$:

$$E[\ell+1,-\ell-1;t,u,v] = (2\ell+1)\;\{E[\ell,-\ell;t-1,u,v]/(2p) + E[\ell,\ell;t,u-1,v]/(2p) +$$

$$+ D_x\; E[\ell,-\ell;t,u,v] + D_y\; E[\ell,\ell;t,u,v] +$$

$$+ (t+1)E[\ell,-\ell;t+1,u,v] + (u+1)E[\ell,\ell;t,u+1,v]\} \qquad \text{C3.6}$$

The same expressions can be used for the recursion in ℓ', $\pm\ell'$.

c) Method of generation

In the use of the recursion formulae C3.3, 5, 6, note that all E coefficients are zero if negative t, u, v arguments are involved, or if t+u+v > $\ell+\ell'$. With this proviso, all E coefficients are easily obtained starting from E[0,0;0,0;0,0,0] = 1 .

First, equations C3.5, 6 allow us to obtain all terms with $|m|=\ell$, $|m'|=\ell'$:

```
loop over ℓ = 1 to L
   recursion in ℓ,±ℓ :
      calculate all E[ℓ,±ℓ;0,0;t,u,v]      (t+u+v≤ℓ)

loop over ℓ' = 1 to L'
   loop over ℓ = 0 to L
      recursion in ℓ',±ℓ' :
         calculate all E[ℓ,±ℓ;ℓ',±ℓ';t,u,v]      (t+u+v≤ℓ+ℓ')
```

where L and L' are the angular quantum numbers of the involved AOs. Next, use of equation C3.3 gives E[ℓ,m;ℓ',m';t,u,v] for $|m|<\ell$ and $|m'|<\ell'$, starting from E[|m|,m;|m'|,m';t,u,v].

C4. Overlap and kinetic integrals

The overlap integrals take the form (see equation C2.6):

$$S_{\omega\omega'} = \int dr\ \chi_\omega\ \chi_{\omega'} = \Sigma_{tuv}\ F[\omega;\omega';t,u,v] \int dr\ \Lambda[p,P;t,u,v] \qquad C4.1$$

Equation C1.9 shows that only the t=u=v=0 integrals are different from zero, so that :

$$S_{\omega\omega'} = F[\omega;\omega';0,0,0]\ (\pi/p)^{3/2} \qquad C4.2$$

For the evaluation of the kinetic integrals we use the relation:

$$-\tfrac{1}{2}\ \nabla^2[X^m_\ell(A;r)\ \exp(-ar_A^2)] = [a(2\ell+3)-2a^2r_A^2]\ X^m_\ell(A;r)\ \exp(-ar_A^2) \qquad C4.3$$

Hence:

$$T_{\omega\omega'} = T_{\omega'\omega} = \int dr\ \chi_{\omega'}\ (-\tfrac{1}{2}\ \nabla^2)\ \chi_\omega = \Sigma_{tuv}\ F[\omega;\omega';t,u,v] \cdot$$
$$\cdot \int dr\ [a(2\ell+3)-2a^2(x_A^2+y_A^2+z_A^2)]\ \Lambda[p,P;t,u,v] \qquad C4.4$$

Use of equation C1.8 (with the substitutions C→A, A→P) for transforming all terms of the type $x_A{}^2\Lambda[P]$ into a linear combination of $\Lambda[P]$ terms reduces all kinetic integrals to overlap ones.

C5. Nuclear attraction integrals

These integrals are of the form :

$$\int dr\ \chi_\omega\ \chi_{\omega'}\ r_C^{-1} = \Sigma_{tuv}\ F[\omega;\omega';t,u,v] \int dr\ \Lambda[p,P;t,u,v]\ r_C^{-1} \qquad C5.1$$

The general integral in the right hand side will be expressed through the symbol:

$$R_o[p,P-C;t,u,v] \equiv R_o[t,u,v] = (p/2\pi) \int dr\ \Lambda[p,P;t,u,v]\ r_C^{-1} \qquad C5.2$$

To calculate these integrals use will be made of the auxiliary functions

$$F_j(w) = \int_o^1 ds\ e^{-ws^2}\ s^{2j} \quad , \qquad C5.3$$

for which powerful algorithms have been developed (see for instance Davidson 1977).

In particular it has been shown by Boys (1950) that

$$R_o[p,D;0,0,0] = F_o(pD^2) \qquad C5.4$$

By using equations C1.1 and C5.2, and after defining D=P-C, we have:

$$R_o[p,D;t,u,v] = \left(\frac{\partial}{\partial P_x}\right)^t \left(\frac{\partial}{\partial P_y}\right)^u \left(\frac{\partial}{\partial P_z}\right)^v (p/2\pi) \int dr\ \Lambda[p,P;0,0,0]\ r_C^{-1} =$$

$$= \left(\frac{\partial}{\partial D_x}\right)^t \left(\frac{\partial}{\partial D_y}\right)^u \left(\frac{\partial}{\partial D_z}\right)^v \int_o^1 ds\ e^{-ps^2D^2} = \int_o^1 ds\ \Lambda[ps^2,D;t,u,v]_o \qquad C5.5$$

where $\Lambda[\ ]_o$ stands for $\Lambda[\ ]$ (as defined in C1.1) at r=0.
Following McMurchie and Davidson,it is convenient at this point to define a more general type of integral:

$$R_j[p,D;t,u,v] = \int_o^1 ds\ (-2ps^2)^j\ \Lambda[ps^2,D;t,u,v]_o \qquad C5.6$$

whence:

$$R_j[p,D;0,0,0] = (-2p)^j\ F_j(pD^2) \qquad C5.7$$

Using the recursion relation C1.6 and dropping the indices p,D gives:

$$R_j[t+1,u,v] = \int_o^1 ds\ (-2ps^2)^{j+1}\ (-D_x\ \Lambda[t,u,v]_o + t\ \Lambda[t-1,u,v]_o) =$$

$$= -D_x\ R_{j+1}[t,u,v] + t\ R_{j+1}[t-1,u,v] \qquad C5.8$$

The required nuclear attraction integrals $I_{tuv} = R_o[t,u,v]$ can then be calculated recursively using the following procedure:

```
Compute R_j[0,0,0] for j=0 to J=ℓ+ℓ'

loop over t = 0 to J
    loop over u = 0 to u_max = J-t
        loop over v = 0 to v_max = J-t-u
            I_tuv = R_o[t,u,v]
            if v=v_max then
                loop over j=0 to v_max-v-1
                    compute R_j[t,u,v+1]  (eq. C5.8)
        if u=u_max then
            loop over j=0 to u_max-u-1
                compute R_j[t,u+1,0]
    if t=J then
        loop over j=0 to J-t-1
            compute R_j[t+1,0,0]
```

C6. Two-electron repulsion integrals

Two-electron repulsion integrals (ERI) involve the Coulomb interaction between two overlap distributions, $\chi_\alpha\ \chi_\beta$ and $\chi_\gamma\ \chi_\delta$, centered in **A**,**B** and **C**,**D**, which may be expanded in HGTFs at centers **P** and **Q** with exponents p and q, respectively.

$$I_{\alpha\beta\gamma\delta} = \int\int dr_1\ dr_2\ \chi_\alpha(r_1)\ \chi_\beta(r_1)\ |r_1-r_2|^{-1}\ \chi_\gamma(r_2)\ \chi_\delta(r_2) =$$

$$= \Sigma_{tuv}\ F[\alpha,\beta;t,u,v]\ \ \Sigma_{t'u'v'}F[\gamma,\delta;t',u',v']\ \cdot$$

$$\cdot\ [t,u,v|r_{12}^{-1}|t',u',v'] \qquad \text{C6.1}$$

where the last quantity is the ERI between $\Lambda[p,P;t,u,v]$ and $\Lambda[q,Q;t',u',v']$. To evaluate these integrals, their translational invariance can be exploited:

$$(\frac{\partial}{\partial P_x})\ [t,u,v|r_{12}^{-1}|t',u',v'] = (-\frac{\partial}{\partial Q_x})\ \ [t,u,v|r_{12}^{-1}|t',u',v'] \qquad \text{C6.2}$$

or, using equation C1.1:

$$[t+1,u,v|r_{12}^{-1}|t',u',v'] = -\ [t,u,v|r_{12}^{-1}|t'+1,u',v'] \qquad \text{C6.3}$$

Similar results hold true for u and v. By repeated applications of equation C6.3 we obtain:

$$[t,u,v|r_{12}^{-1}|t',u',v'] = (-1)^{t'+u'+v'}[t+t',u+u',v+v'|r_{12}^{-1}|0,0,0] \qquad \text{C6.4}$$

It must be noticed that the number of integrals to be computed for the calculation of $I_{\alpha\beta\gamma\delta}$ may be much lower if use is made of the right hand side instead of the left hand side of equation C6.4.

The way of proceeding from this point on is very similar to the one for the nuclear attraction integrals. We start from the relation existing between the basic integral C6.4 and the F_o function introduced in eq. C5.4 (Boys 1950):

$$[0,0,0|r_{12}^{-1}|0,0,0] = 2\ \pi^{5/2}\ p^{-1}\ q^{-1}\ (p+q)^{-1/2}\ F_o(w) \qquad \text{C6.5}$$

$$w = e\ (P-Q)^2 \qquad \text{C6.6}$$

$$e = pq/(p+q) \qquad \text{C6.7}$$

From equations C1.1, C5.2 and C5.4 we obtain :

$$[t,u,v|r_{12}^{-1}|0,0,0] = 2\pi^{5/2}p^{-1}q^{-1}\ (p+q)^{-1/2}\ (\frac{\partial}{\partial P_x})^t\ (\frac{\partial}{\partial P_y})^u\ (\frac{\partial}{\partial P_z})^v\ F_o(w) =$$

$$= 2\ \pi^{5/2}\ p^{-1}\ q^{-1}\ (p+q)^{-1/2}\ R_o[e,P-Q;t,u,v] \qquad \text{C6.8}$$

The generation of the $R_o[t,u,v]$ functions can be accomplished exactly in the same way as explained in section C5. In summary we have :

$$I_{\alpha\beta\gamma\delta} = 2\,\pi^{5/2}p^{-1}q^{-1}(p+q)^{-1/2}\,\Sigma_{tuv}\,F[\alpha,\beta;t,u,v]\,\Sigma_{t'u'v'}F[\gamma,\delta;t',u',v']\cdot$$

$$\cdot\,(-1)^{t'+u'+v'}\;\;R_o[e,P-Q;t+t',u+u',v+v'] \qquad \text{C6.9}$$

APPENDIX D. SYMBOLS AND NOTATIONS

This appendix is intended to facilitate the interpretation of symbols, conventions and acronyms occurring in this book.

Note that:

Atomic units (a.u.) are used throughout; for the main quantities of interest the value in SI units is:

Length	a_0	5.2918×10^{-11}	m
Mass	m_0	9.1096×10^{-31}	kg
Charge	e	1.6022×10^{-18}	C
Angular momentum	$\hbar$	1.0546×10^{-34}	J s
Energy	ϵ_0	4.3598×10^{-18}	J
Time	$\hbar/\epsilon_0$	2.4189×10^{-17}	s
Electric potential	ϵ_0/e	2.7211×10^{1}	V
Electric dipole moment	ea_0	8.4784×10^{-30}	C m
Electric charge density	$e/a^3{}_0$	1.0812×10^{12}	C m^{-3}

Bold characters refer to three-dimensional vectors or matrices; their components and elements are typed unboldened and with subscript indices.

For typographical clarity superscript and subscript indices are nearer to the reference line when they appear in the text; they are therefore typed on adjoining columns to avoid superposition of the characters. So, for instance:

p^{g}_{12} appears in the text as $p^{g}{}_{12}$

$X^{\pm m}_{\varrho}$ appears in the text as $X_{\varrho}{}^{\pm m}$

In the following list of acronyms the symbol in parentheses, when present, refers to the section where the corresponding term is introduced or explained in detail.

AF	Autocorrelation function	(III.4a,c)
AO	Atomic Orbital	(I.1,I.2c,II.2d)
APW	Augmented Plane Wave	(I.1,I.2c)
BF	Bloch Function	(I.2.c,II.2a)
BS	Basis Set	(I.3b)
BZ	Brillouin Zone	(App. B)
CI	Configuration Interaction	(I.1)
CO	Crystalline Orbital	(I.2c)
COHSEX	Coulomb Hole plus Screened Exchange	(I.3f)
CP(F)	Compton Profile (function)	(III.4a)
CSF	Colle & Salvetti Functional	(I.3f)
CS	Configuration Space	(I.2d)
DF	Density Functional	(I.2b)
DOS	Density of States	(II.6)
EMD(F)	Electron Momentum Distribution (Function)	(III.4a)
ERI	Electron Repulsion Integral	(App. C6)
GF	Green Function	(I.2d)
GTO	Gaussian Type Orbital	(II.2a)
HF	Hartree-Fock	
HGTF	Hermite Gaussian Type Functions	(App. C1)
IBZ	Irreducible part of the Brillouin Zone	(App.B)

IR	Irreducible Representation	(App.B)
KKR	Korringa-Kohn-Rostoker	(I.2a)
LAPW	Linearized Augmented Plane Wave	(I.2c)
LCAO	Linear Combination of Atomic Orbitals	(I.1)
LD(F)	Local Density (Functional)	(I.2b)
MO	Molecular Orbital	(I.1)
MS	Momentum Space	(I.2d)
MT	Muffin Tin	(I.2a)
PP	Pseudopotential	(I.2b,I.3g)
PW	Plane Wave	(I.1,I.2c)
SC(F)	Self Consistent (Field)	(II.3)
SPW	Symmetrized Plane Waves	(II.6a)
SCF	Self Consistent Field	(I.1)
STO-nG	Slater Type Orbitals- n contracted Gaussians	(I.3b)
TB	Tight Binding	(I.1)

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