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Commentationes

Applications of Fourier Transforms in Molecular Orbital Theory. Calculation of Optical Properties and Tables of Two-Center One-Electron Integrals

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Fourier transform methods initiated by Geller and Harris are applied to the calculation of optical properties of molecules. Tables of one-electron two-center integrals needed for the accurate computation of molecular absorption and optical activity are calculated by the Fourier transform method. A general theorem is derived which allows the angular part of the integrals to be treated by means of projection operators. The radial parts of the integrals are treated by the methods of Harris. The results are obtained in a simple closed form which avoids the usual transformation to local coordinates. The two-center integrals evaluated include matrix elements of the momentum operator, the dipole moment operator, the tensor operator $x_\mu \frac{\partial}{\partial x_\nu}$, the quadrupole moment operator, and the angular momentum operator. These are evaluated between $1s$, $2s$, and $2p$ Slater-type atomic orbitals located on different atoms. The results are expressed as functions of the Slater exponents and of the relative coordinates of the two atoms.

Key words: Two-center one-electron integrals – Fourier transforms in MO theory – Optical properties

Introduction

In order to calculate the optical properties of molecules (including oscillator strengths, linear dichroism, circular dichroism, optical rotatory dispersion and photon scattering cross sections), from a knowledge of the molecular orbitals [1–6], one needs to evaluate matrix elements of the form:

$$(M_{st})_\nu = \int d^3x\, \Phi_s(\boldsymbol{x})\, e^{i\boldsymbol{\varkappa}\cdot\boldsymbol{x}} \frac{\partial}{\partial x_\nu} \Phi_t(\boldsymbol{x}) \qquad \nu = 1, 2, 3\,. \tag{1}$$

Here $\boldsymbol{\varkappa}$ is the photon wave number, while Φ_s and Φ_t are molecular orbitals. If we let $\boldsymbol{X}_j$ represent the position of the jth atom in a molecule, while $\chi_n(\boldsymbol{x}-\boldsymbol{X}_j)$ represents an atomic orbital of type n localized in the jth atom, then the molecular orbitals can be written in the form:

$$\Phi_s(\boldsymbol{x}) = \sum_{n,j} \chi_n(\boldsymbol{x}-\boldsymbol{X}_j)\, C_{nj,s}\,. \tag{2}$$

If we expand $\exp(i\boldsymbol{\varkappa}\cdot\boldsymbol{x})$ in a Taylor series, retaining only the first two terms, then (1) and (2) can be combined to yield:

$$
\begin{aligned}
(M_{s,t})_\nu &= \int d^3x\,\Phi_s(\boldsymbol{x})\,e^{i\boldsymbol{\varkappa}\cdot\boldsymbol{x}}\frac{\partial}{\partial x_\nu}\Phi_t(\boldsymbol{x}) \\
&= \sum_{n'j',nj} C_{n'j',s}C_{nj,t}\Bigg[(1+i\boldsymbol{\varkappa}\cdot\boldsymbol{X}_{j'})\,\{F_{n'n}(\boldsymbol{R}_{j'j})\}_\nu \\
&\quad + i\sum_{\mu=1}^{3}\varkappa_\mu\{T_{n'n}(\boldsymbol{R}_{j'j})\}_{\mu\nu}\Bigg]
\end{aligned}
\tag{3}
$$

where

$$
\{F_{n'n}(\boldsymbol{R}_{j'j})\}_\nu \equiv \int d^3x\,\chi_{n'}(\boldsymbol{x}-\boldsymbol{X}_{j'})\frac{\partial}{\partial x_\nu}\chi_n(\boldsymbol{x}-\boldsymbol{X}_j)
\tag{4}
$$

and

$$
\{T_{n'n}(\boldsymbol{R}_{j'j})\}_{\mu\nu} \equiv \int d^3x\,\chi_{n'}(\boldsymbol{x}-\boldsymbol{X}_{j'})\,(\boldsymbol{x}-\boldsymbol{X}_{j'})_\mu\frac{\partial}{\partial x_\nu}\chi_n(\boldsymbol{x}-\boldsymbol{X}_j).
\tag{5}
$$

For the evaluation of oscillator strengths, only the term

$$
\lim_{\boldsymbol{\varkappa}\Rightarrow 0}\{(M_{s,t})_\nu\} = \int d^3x\,\Phi_s(\boldsymbol{x})\frac{\partial}{\partial x_\nu}\Phi_t(\boldsymbol{\varkappa})
\tag{6}
$$

is necessary, while the terms up to first order in $\boldsymbol{\varkappa}$ are needed for the calculation of circular dichroism and optical rotatory dispersion. The matrix element of the momentum operator (6), is often converted into a matrix element of the dipole moment operator by means of the relation:

$$
\int d^3x\,\Phi_s(\boldsymbol{x})\frac{\partial}{\partial x_\nu}\Phi_t(\boldsymbol{x}) = \frac{m(E_t-E_s)}{\hbar^2}\int d^3x\,\Phi_s(\boldsymbol{x})\,x_\nu\,\Phi_t(\boldsymbol{x}).
\tag{7}
$$

However, as has been pointed out by a number of authors [7–21], who have concerned themselves with matrix elements of the form (4)–(6), Eq. (7) is only an exact relation if we are dealing with exact solutions of the Schrödinger equation. In cases where the wave functions are only approximate, the use of (7) can lead to very large errors. Therefore it is of interest to evaluate matrix elements of the momentum operator (6) directly without converting it to the dipole moment by means of (7). The authors who have evaluated (6) directly do so by using an ellipsoidal coordinate system [22–23]. The ellipsoidal coordinate method for evaluating two-center one-electron integrals is rather cumbersome, and it is necessary, when using this method, to transform to a local coordinate system oriented along the line joining the two atoms. We shall instead evaluate the matrix elements by means of the Fourier transform methods pioneered by Geller and Harris, making use of the radial integrals studied by them. The Fourier transform method leads to a simple analytic evaluation of all the two-center one-electron integrals. Besides the simple closed form of the results, the Fourier transform method for calculating optical properties of molecules has the great advantage that it avoids the transformation to local coordinates.

The Fourier Transform Method for Calculating Two-Center One-Electron Integrals

Let $\alpha_n(\boldsymbol{k})$ be the Fourier transform of the atomic orbital $\chi_n(\boldsymbol{x})$, so that

$$\chi_n(\boldsymbol{x}) = \int d^3 k \exp(i\boldsymbol{k}\cdot\boldsymbol{x})\,\alpha_n(\boldsymbol{k}) \tag{8}$$

and

$$\alpha_n(\boldsymbol{k}) = \frac{1}{(2\pi)^3}\int d^3 x \exp(-i\boldsymbol{k}\cdot\boldsymbol{x})\,\chi_n(\boldsymbol{x})\,. \tag{9}$$

Then

$$\chi_n(\boldsymbol{x}-\boldsymbol{X}_j) = \int d^3 k \exp[i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{X}_j)]\,\alpha_n(\boldsymbol{k}) \tag{10}$$

and

$$\chi_{n'}(\boldsymbol{x}-\boldsymbol{X}_{j'}) = \int d^3 k' \exp[i\boldsymbol{k}'\cdot(\boldsymbol{x}-\boldsymbol{X}_{j'})]\,\alpha_{n'}(\boldsymbol{k}')\,. \tag{11}$$

Substituting (10) and (11) into (4), we obtain:

$$\begin{aligned}
(F_{n'n})_\nu &= \int d^3 x \chi_{n'}(\boldsymbol{x}-\boldsymbol{X}_{j'}) \frac{\partial}{\partial x_\nu}\chi_n(\boldsymbol{x}-\boldsymbol{X}_j)\\
&= \int d^3 x \int d^3 k \int d^3 k' \exp[i\boldsymbol{k}'\cdot(\boldsymbol{x}-\boldsymbol{X}_{j'})]\,\alpha_{n'}(\boldsymbol{k}')\frac{\partial}{\partial x_\nu}\exp[i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{X}_j)]\,\alpha_n(\boldsymbol{k})\\
&= \int d^3 k \int d^3 k' \exp[-i(\boldsymbol{k}'\cdot\boldsymbol{X}_{j'}+\boldsymbol{k}\cdot\boldsymbol{X}_j)\,\alpha_{n'}(\boldsymbol{k}')\,ik_\nu\alpha_n(\boldsymbol{k})\\
&\quad\cdot\int d^3 x \exp[i(\boldsymbol{k}+\boldsymbol{k}')\cdot\boldsymbol{x}]\,.
\end{aligned} \tag{12}$$

Then, since

$$\int d^3 x \exp[i(\boldsymbol{k}+\boldsymbol{k}')\cdot\boldsymbol{x}] = (2\pi)^3\,\delta(\boldsymbol{k}+\boldsymbol{k}') \tag{13}$$

we have

$$\begin{aligned}
(F_{n'n})_\nu &\equiv \int d^3 x \chi_{n'}(\boldsymbol{x}-\boldsymbol{X}_{j'}) \frac{\partial}{\partial x_\nu}\chi_n(\boldsymbol{x}-\boldsymbol{X}_j)\\
&= (2\pi)^3 \int d^3 k \exp(i\boldsymbol{k}\cdot\boldsymbol{R})\,\alpha_{n'}(-\boldsymbol{k})\,ik_\nu\alpha_n(\boldsymbol{k})
\end{aligned} \tag{14}$$

where

$$\boldsymbol{R} \equiv \boldsymbol{X}_{j'} - \boldsymbol{X}_j\,. \tag{15}$$

In a similar way, we obtain the relations:

$$\begin{aligned}
(G_{n'n})_\nu &\equiv \int d^3 x \chi_{n'}(\boldsymbol{x}-\boldsymbol{X}_{j'})\,(\boldsymbol{x}-\boldsymbol{X}_j)_\nu\,\chi_n(\boldsymbol{x}-\boldsymbol{X}_j)\\
&= (2\pi)^3 \int d^3 k \exp(i\boldsymbol{k}\cdot\boldsymbol{R})\,\alpha_{n'}(-\boldsymbol{k})\,\{\beta_n(\boldsymbol{k})\}_\nu
\end{aligned} \tag{16}$$

where

$$\{\beta_n(\boldsymbol{k})\}_\nu \equiv \frac{1}{(2\pi)^3}\int d^3 x \exp(-i\boldsymbol{k}\cdot\boldsymbol{x})\,x_\nu\chi_n(\boldsymbol{x}) \tag{17}$$

$$\begin{aligned}
S_{n'n} &\equiv \int d^3 x \chi_{n'}(\boldsymbol{x}-\boldsymbol{X}_{j'})\,\chi_n(\boldsymbol{x}-\boldsymbol{X}_j)\\
&= (2\pi)^3 \int d^3 k \exp(i\boldsymbol{k}\cdot\boldsymbol{R})\,\alpha_{n'}(-\boldsymbol{k})\,\alpha_n(\boldsymbol{k})
\end{aligned} \tag{18}$$

$$\begin{aligned}
(T_{n'n})_{\mu\nu} &\equiv \int d^3 x \chi_{n'}(\boldsymbol{x}-\boldsymbol{X}_{j'})\,(\boldsymbol{x}-\boldsymbol{X}_{j'})_\mu \frac{\partial}{\partial x_\nu}\chi_n(\boldsymbol{x}-\boldsymbol{X}_j)\\
&= (2\pi)^3 \int d^3 k \exp(i\boldsymbol{k}\cdot\boldsymbol{R})\,\{\beta_{n'}(-k)\}_\mu\,ik_\nu\alpha_n(\boldsymbol{k})
\end{aligned} \tag{19}$$

and

$$\begin{aligned}
(Q_{n'n})_{\mu\nu} &\equiv \int d^3 x \chi_{n'}(\boldsymbol{x}-\boldsymbol{X}_{j'})\,(\boldsymbol{x}-\boldsymbol{X}_{j'})_\mu\,(\boldsymbol{x}-\boldsymbol{X}_j)_\nu\,\chi_n(\boldsymbol{x}-\boldsymbol{X}_j)\\
&= (2\pi)^3 \int d^3 k \exp(i\boldsymbol{k}\cdot\boldsymbol{R})\,\{\beta_{n'}(-\boldsymbol{k})\}_\mu\,\{\beta_n(\boldsymbol{k})\}_\nu\,.
\end{aligned} \tag{20}$$

Fourier Transforms of Atomic Orbitals

In order to evaluate the Fourier transforms $\alpha_n(\boldsymbol{k})$ and $\{\beta_n(\boldsymbol{k})\}_\nu$ defined by (8) and (17), we make use of the expansion:

$$\exp(-i\boldsymbol{k}\cdot\boldsymbol{x}) = 4\pi \sum_{l=0}^{\infty} (-i)^l j_l(kr) \sum_{m=-l}^{l} Y_{lm}^*(\theta,\varphi)\, Y_{lm}(\theta_k,\varphi_k) \tag{21}$$

where j_l is a spherical Bessel function of order l (26). k, θ_k, and φ_k are the spherical polar coordinates of the vector $\boldsymbol{k}$ in reciprocal space. If χ_n is a Slater-type orbital of the form:

$$\chi_{nlm}(\boldsymbol{x}) = \sqrt{\frac{(2\zeta)^{2n+1}}{(2n)!}}\, r^{n-1} \exp(-\zeta r)\, Y_{lm}(\theta,\varphi) \tag{22}$$

then substituting (22) and (21) into (9) and making use of the orthonormality of the spherical harmonics, we obtain:

$$\alpha_{nlm}(\boldsymbol{k}) = \sqrt{\frac{(2\zeta)^{2n+1}}{(2n)!}}\, \frac{(-i)^l}{2\pi^2} J_{n+1,l}(k)\, Y_{lm}(\theta_k,\varphi_k) \tag{23}$$

where

$$J_{\mu\nu} \equiv \int_0^{\infty} dr\, r^{\mu} j_\nu(kr) \exp(-\zeta r). \tag{24}$$

The integrals $J_{\mu\nu}$ have been studied by Geller [29, 30] and Harris [25]. They can be evaluated directly by inserting the explicit expression for $j_\nu(kr)$ and integrating. Alternatively, they can be generated by means of the recursion formulae given by Harris:

$$\begin{aligned} J_{\nu+1,\nu} &= \left(\frac{2\nu k}{k^2+\zeta^2}\right) J_{\nu,\nu-1} \\ J_{\nu+2,\nu} &= \frac{(2\nu+2)\zeta}{(k^2+\zeta^2)} J_{\nu+1,\nu} \\ (k^2+\zeta^2) J_{\mu+1,\nu} + (\mu+\nu)(\mu-\nu-1) J_{\mu-1,\nu} &= 2\mu\zeta J_{\mu\nu} \\ k J_{\mu,\nu-1} + (\mu-\nu-1) J_{\mu-1,\nu} &= \zeta J_{\mu\nu}\,. \end{aligned} \tag{25}$$

Starting with

$$J_{1,0} = \frac{1}{k^2+\zeta^2} \tag{26}$$

and using the recursion relations of Harris (25), we obtain the functions shown in Table 1. Substitution into (23) yields the following Fourier transforms for the real Slater-type orbitals up to $n=2$:

$$\begin{aligned} \alpha_{1s} &= \left(\frac{\zeta}{\pi}\right)^{5/2} \frac{1}{(k^2+\zeta^2)^2} \\ \alpha_{2s} &= \left(\frac{\zeta}{\pi}\right)^{5/2} \frac{(3\zeta^2-k^2)}{\sqrt{3}(k^2+\zeta^2)^3} \\ \alpha_{2p_\mu} &= -4\pi i \left(\frac{\zeta}{\pi}\right)^{7/2} \frac{k}{(k^2+\zeta^2)^3} \frac{k_\mu}{k}\,. \end{aligned} \tag{27}$$

Table 1.

$$J_{\mu\nu} = \int_0^\infty dr\, r^\mu j_\nu(kr)\, e^{-\zeta r}$$

$\nu \uparrow$				
3				$\frac{48k^3}{(k^2+\zeta^2)^4}$
2			$\frac{8k^2}{(k^2+\zeta^2)^3}$	$\frac{48k^2\zeta}{(k^2+\zeta^2)^4}$
1		$\frac{2k}{(k^2+\zeta^2)^2}$	$\frac{8k\zeta}{(k^2+\zeta^2)^3}$	$\frac{8k(5\zeta^2-k^2)}{(k^2+\zeta^2)^4}$
0	$\frac{1}{(k^2+\zeta^2)}$	$\frac{2\zeta}{(k^2+\zeta^2)^2}$	$\frac{2(3\zeta^2-k^2)}{(k^2+\zeta^2)^3}$	$\frac{24\zeta(\zeta^2-k^2)}{(k^2+\zeta^2)^4}$
	1	2	3	4 $\mu\rightarrow$

In a similar way we can generate the functions defined by Eq. (17)

$$\begin{aligned}
(\beta_{1s})_\mu &= -i\left(\frac{\zeta}{\pi}\right)^{5/2} \frac{4k}{(k^2+\zeta^2)^3}\frac{k_\mu}{k} \\
(\beta_{2s})_\mu &= \frac{-4i}{\sqrt{3}}\left(\frac{\zeta}{\pi}\right)^{5/2} \frac{k(5\zeta^2-k^2)}{(k^2+\zeta^2)^4}\frac{k_\mu}{k} \\
(\beta_{2p_\mu})_\nu &= \frac{4\zeta^{7/2}}{\pi^{5/2}}\left\{\frac{\delta_{\mu\nu}}{(k^2+\zeta^2)^3} - \frac{6k_\mu k_\nu}{(k^2+\zeta^2)^4}\right\}.
\end{aligned} \tag{28}$$

Angular Momentum Projection Operators Acting on Tensor Functions

Before proceeding further with the evaluation of the two-center one-electron integrals of Eqs. (14)–(20), it is convenient to notice the following general property of three-dimensional Fourier transforms: Suppose that we have a function which can be expressed as a product of a radial part $A(k)$ and an angular part $f(\theta_k, \varphi_k)$. Then, from the expansion

$$\exp(i\boldsymbol{k}\cdot\boldsymbol{R}) = 4\pi \sum_{l=0}^{\infty} i^l j_l(kR) \sum_{m=-l}^{l} Y_{lm}^*(\theta_k, \varphi_k)\, Y_{lm}(\theta_R, \varphi_R) \tag{29}$$

it follows that

$$\int d^3k \exp(i\boldsymbol{k}\cdot\boldsymbol{R})\, A(k)\, f(\theta_k, \varphi_k) = \sum_{l=0}^{\infty} a_l(R)\, O_l\{f(\theta_R, \varphi_R)\} \tag{30}$$

where

$$a_l(R) \equiv 4\pi i^l \int_0^\infty dk\, k^2 j_l(kR)\, A(k) \tag{31}$$

and

$$O_l\{f(\theta_R, \varphi_R)\} \equiv \sum_{m=-l}^{l} Y_{lm}(\theta_R, \varphi_R) \int d\Omega_k Y_{lm}^*(\theta_k, \varphi_k)\, f(\theta_k, \varphi_k)\,. \tag{32}$$

In Eq. (32), $O_l\{f(\theta_R, \varphi_R)\}$ is just that component of the angular function $f(\theta_R, \varphi_R)$ which transforms under rotations according to the angular momentum quantum number l. In other words, O_l is a weak projection operator which annihilates all of the components of $f(\theta_R, \varphi_R)$ except that part which corresponds to angular momentum l. If we have some other means of finding the effect of such a projection operator on $f(\theta_R, \varphi_R)$, then we need not evaluate the integral (32).

Looking at (27) and (28), we can see that the angular functions which occur in the integrals (14)–(20) are tensor of the form:

$$f(\theta_k, \varphi_k) = \frac{\overbrace{k_\mu k_\nu \dots k_\sigma}^{N \text{ factors}}}{k^N} \qquad \mu, \nu, \dots \sigma \dots 1, 2, 3\,. \tag{33}$$

Thus, in our case, (30) takes on the particular form:

$$\begin{aligned} &\int d^3k \exp(i\boldsymbol{k}\cdot\boldsymbol{R})\, A(k) \frac{k_\mu k_\nu \dots k_\sigma}{k^N} \\ &\qquad = \sum a_l(R)\, O_l\left(\frac{R_\mu R_\nu \dots R_\sigma}{R^N}\right) \\ &l = 0, 2, 4, \dots N\ (N \text{ even}) \\ &l = 1, 3, 5, \dots N\ (N \text{ odd}) \qquad \mu, \nu, \dots \sigma = 1, 2, 3\,. \end{aligned} \tag{34}$$

The even values of l enter the sum when N is even, and the odd values enter when N is odd because if this were not the case, we would not be able to maintain the identity

$$\frac{R_\mu R_\nu \dots R_\sigma}{R^N} = \sum_l O_l\left(\frac{R_\mu R_\nu \dots R_\sigma}{R^N}\right)$$

when both sides of the equation are subjected to the inversion operation $\boldsymbol{R} \Rightarrow -\boldsymbol{R}$. The series in (34) terminates at N for the following reason: The usual theory of angular momentum tells us that the maximum value of angular momentum which can result from coupling l and l' is $l+l'$. Since R_μ/R and R_ν/R each correspond to $l=1$, the maximum value of angular momentum can be contained in the direct product $R_\mu R_\nu/R^2$ is $l+l'=1+1=2$. Similarly, when $R_\mu R_\nu/R^2$ and R_σ/R are coupled to yield $R_\mu R_\nu R_\sigma/R^3$, the maximum value of angular momentum which can be contained in the direct product is $2+1=3$. Proceeding in this way, we find that if N is the rank of the tensor function, then

$$O_l\left(\frac{R_\mu R_\nu \dots R_\sigma}{R^N}\right) = 0 \quad \text{for} \quad l > N\,.$$

Using a table of spherical harmonics, or alternatively, using Löwdin's projection operator methods, we can construct the angular functions

$$O_l\left(\frac{R_\mu R_\nu \dots R_\sigma}{R^N}\right)$$

Table 2.

$$O_1\left(\frac{R_\mu}{R}\right) = \frac{R_\mu}{R}$$

$$O_2\left(\frac{R_\mu R_\nu}{R^2}\right) = \frac{R_\mu R_\nu}{R^2} - \frac{\delta_{\mu\nu}}{3}$$

$$O_0\left(\frac{R_\mu R_\nu}{R^2}\right) = \frac{\delta_{\mu\nu}}{3}$$

$$O_3\left(\frac{R_\mu R_\nu R_\sigma}{R^3}\right) = \begin{cases} \dfrac{R_\mu R_\nu R_\sigma}{R^3} & \mu \neq \nu \neq \sigma \neq \mu \\ \dfrac{R_\mu R_\mu R_\sigma}{R^3} - \dfrac{R_\sigma}{5R} & \mu = \nu \neq \sigma \\ \dfrac{R_\mu R_\mu R_\mu}{R^3} - \dfrac{3R_\mu}{5R} & \mu = \nu = \sigma \end{cases}$$

$$O_1\left(\frac{R_\mu R_\nu R_\sigma}{R^3}\right) = \begin{cases} 0 & \mu \neq \nu \neq \sigma \neq \mu \\ \dfrac{R_\sigma}{5R} & \mu = \nu \neq \sigma \\ \dfrac{3R_\mu}{5R} & \mu = \nu = \sigma \end{cases}$$

$$O_4\left(\frac{R_\mu R_\mu R_\nu R_\sigma}{R^4}\right) = \begin{cases} \dfrac{R_\mu R_\mu R_\nu R_\sigma}{R^4} - \dfrac{R_\nu R_\sigma}{7R^2} & \mu \neq \nu \neq \sigma \neq \mu \\ \dfrac{R_\mu R_\mu R_\mu R_\sigma}{R^4} - \dfrac{3R_\mu R_\sigma}{7R^2} & \mu = \nu \neq \sigma \\ \dfrac{R_\mu R_\mu R_\nu R_\nu}{R^4} - \dfrac{R_\mu R_\mu + R_\nu R_\nu}{7R^2} + \dfrac{1}{35} & \mu \neq \nu = \sigma \\ \dfrac{R_\mu R_\mu R_\mu R_\mu}{R^4} - \dfrac{6R_\mu R_\mu}{7R^2} + \dfrac{3}{35} & \mu = \nu = \sigma \end{cases}$$

$$O_2\left(\frac{R_\mu R_\mu R_\nu R_\sigma}{R^4}\right) = \begin{cases} \dfrac{R_\nu R_\sigma}{7R^2} & \mu \neq \nu \neq \sigma \neq \mu \\ \dfrac{3R_\mu R_\sigma}{7R^2} & \mu = \nu \neq \sigma \\ \dfrac{R_\mu R_\mu + R_\nu R_\nu}{7R^2} - \dfrac{2}{21} & \mu \neq \nu = \sigma \\ \dfrac{6R_\mu R_\mu}{7R^2} - \dfrac{2}{7} & \mu = \nu = \sigma \end{cases}$$

$$O_0\left(\frac{R_\mu R_\mu R_\nu R_\sigma}{R^4}\right) = \begin{cases} 0 & \mu \neq \nu \neq \sigma \neq \mu \\ 0 & \mu = \nu \neq \sigma \\ \frac{1}{15} & \mu \neq \nu = \sigma \\ \frac{1}{5} & \mu = \nu = \sigma \end{cases}$$

as shown in Table 2. For example, looking at a table of spherical harmonics, we see that

$$Y_{2,0} \sim 3\cos^2\theta - 1 = 3\frac{ZZ}{R^2} - 1\,.$$

Therefore

$$O_0\left(\frac{3ZZ}{R^2} - 1\right) = 0 \quad \text{and} \quad O_0\left(\frac{ZZ}{R^2}\right) = \frac{1}{3}\,.$$

However, we know that

$$O_0\left(\frac{ZZ}{R^2}\right) + O_2\left(\frac{ZZ}{R^2}\right) = \frac{ZZ}{R^2}\,,$$

and therefore it follows that

$$O_2\left(\frac{ZZ}{R^2}\right) = \frac{ZZ}{R^2} - \frac{1}{3}\,.$$

Proceeding in this way, we can construct the angular functions of Table 2.

The Radial Functions of Geller and Harris

From (34) we can see that the one-electron two-center integrals can be expressed in terms of the angular functions of Table 2 and in terms of the radial integrals:

$$a_l(R) = 4\pi i^l \int_0^\infty dk\,k^2 j_l(kR)\,A(k) \tag{35}$$

where $A(k)$ represents the radial part of the expressions occurring in Eqs. (14)–(20). For example, combining (14), (27), and (34), we have:

$$(F_{2p_\mu,2p_\nu})_\sigma = \sum_{l=1,3} a_l(R)\,O_l\left(\frac{R_\mu R_\nu R_\sigma}{R^3}\right) \tag{36}$$

where

$$a_l(R) = 4\pi i^l \int dk\,k^2 j_l(kR)\left\{(2\pi)^3\left(\frac{\zeta_1}{\pi}\right)^{7/2}\frac{(4\pi ik)\,(ik)}{(k^2+\zeta_1^2)^3}\left(\frac{\zeta_2}{\pi}\right)^{7/2}\frac{(-4\pi ik)}{(k^2+\zeta_2^2)^3}\right\} \tag{37}$$

Radial integrals of this type have been studied by Geller [29, 30] and Harris [25]. They introduce the notation:

$$W_{i,i'}^{l,j} \equiv \frac{2}{\pi}\int_0^\infty \frac{dk\,k^{l+2j} j_l(kR)}{(k^2+\zeta_1^2)^i\,(k^2+\zeta_2^2)^{i'}} \tag{38}$$

Thus, using Harris' notation, we can write:

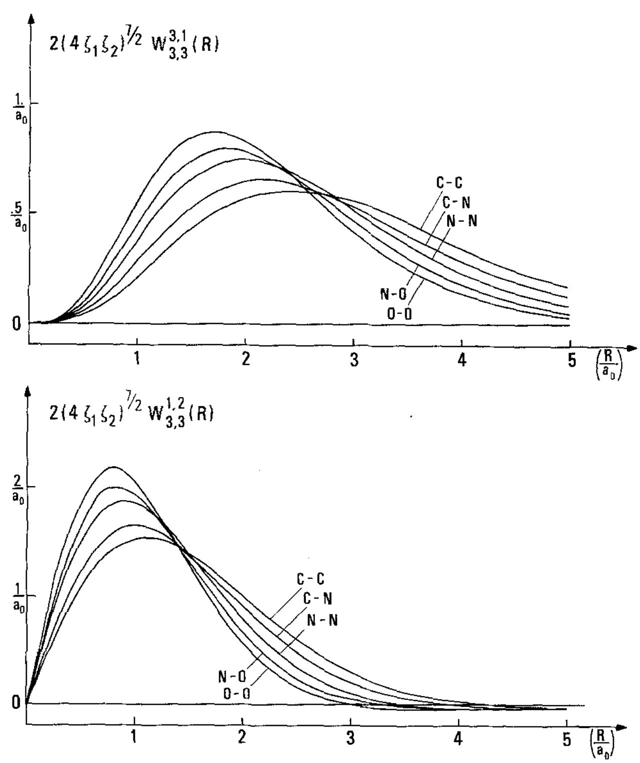
$$(F_{2p_\mu,2p_\nu})_\sigma = 2(4\zeta_1\zeta_2)^{7/2}\,i\sum_{l=1,3} i^l W_{3,3}^{l,\left(\frac{5-l}{2}\right)} O_l\left(\frac{R_\mu R_\nu R_\sigma}{R^3}\right) \tag{39}$$

The radial integrals $W_{i,i'}^{l,j}$ can be evaluated directly by contour integration. However, this direct method of evaluating $W_{i,i'}^{l,j}$ is extremely tedious. Harris instead evaluates these integrals by a very elegant procedure using recursion relations and using the relation [31]:

$$W_{S+1,0}^{l,1} = \frac{R^S}{2^S S!\,\zeta_1^{S-l-1}}\, k_{S-l-1}(\zeta_1 R) \tag{40}$$

where $k_n(x)$ is a modified spherical Bessel function of order n:

$$\begin{aligned}
k_{-1}(x) &= \frac{1}{x}\, e^{-x} \\
k_0(x) &= \frac{1}{x}\, e^{-x} \\
k_1(x) &= \left(\frac{1}{x^2} + \frac{1}{x}\right) e^{-x} \\
k_2(x) &= \left(\frac{3}{x^3} + \frac{3}{x^2} + \frac{1}{x}\right) e^{-x} \\
k_3(x) &= \left(\frac{15}{x^4} + \frac{15}{x^3} + \frac{6}{x^2} + \frac{1}{x}\right) e^{-x} \\
&\vdots \\
&\text{etc.}
\end{aligned} \tag{41}$$



Figs. 1 and 2. These figures show the radial functions which are needed for the accurate evaluation of oscillator strengths in $\pi \to \pi^*$ transitions, [see Eqs. (4), (38), and (39)]. The curves were evaluated using the Slater exponents given by Clementi and Riamondi [28] for nitrogen, carbon and oxygen

The modified spherical Bessel functions $k_n(x)$ obey the recursion relations:

$$-\frac{1}{x^n}k_{n+1}=\frac{d}{dx}\left[\frac{k_n}{x^n}\right]. \tag{42}$$

The radial functions $W_{i,i'}^{l,j}$ obey the recursion relations:

$$(\zeta_2^2-\zeta_1^2)\,W_{i,i'}^{l,j}=W_{i,i'-1}^{l,j}-W_{i-1,i'}^{l,j} \tag{43}$$

$$\left(\frac{2l+1}{R}\right)W_{i,i'}^{l,j}=W_{i,i'}^{l+1,j}+W_{i,i'}^{l-1,j+1}. \tag{44}$$

Starting with (40), one can use (43) and (44) to advance the indices of $W_{i,i'}^{l,j}$ and in this way one obtains the desired function. Harris also discusses a procedure which can be used to evaluate $W_{i,i'}^{l,j}$ in the case where ζ_1 and ζ_2 are almost equal, and (43) is no longer computationally feasible. Examples of the radial functions are shown in Figs. 1 and 2.

Tables of One-Electron Two-Center Integrals

Having discussed both the angular and radial parts of the integrals in Eqs. (14)–(20), we are now in a position to evaluate them by a straightforward application of Eqs. (34), (31), (27), and (28). The results, expressed in terms of the

Table 3. Integrals involving the momentum operator

$$(F_{n'n})_\mu\equiv\int d^3x\,\chi_{n'}(\boldsymbol{x}-\boldsymbol{X}_{j'})\frac{\partial}{\partial x_\mu}\chi_n(\boldsymbol{x}-\boldsymbol{X}_j)$$

$$\boldsymbol{R}=\boldsymbol{X}_{j'}-\boldsymbol{X}_j$$

$$(F_{1s,1s})_\mu=-\frac{1}{2}(4\zeta_1\zeta_2)^{5/2}\,W_{2,2}^{1,1}\frac{R_\mu}{R}$$

$$(F_{1s,2s})_\mu=\frac{-(4\zeta_1\zeta_2)^{5/2}}{2\sqrt{3}}(3\zeta_2^2\,W_{2,3}^{1,1}-W_{2,3}^{1,2})\frac{R_\mu}{R}$$

$$(F_{2s,2s})_\mu=\frac{-(4\zeta_1\zeta_2)^{5/2}}{6}\{9\zeta_1^2\zeta_2^2\,W_{3,3}^{1,1}-3(\zeta_1^2+\zeta_2^2)\,W_{3,3}^{1,2}+W_{3,3}^{1,3}\}\frac{R_\mu}{R}$$

$$(F_{1s,2p_\mu})_\nu=(2\zeta_1)^{5/2}(2\zeta_2)^{7/2}\sum_{l=0,2}i^l\,W_{2,3}^{l,\left(\frac{4-l}{2}\right)}\,O_l\left(\frac{R_\mu R_\nu}{R^2}\right)$$

$$(F_{2s,2p_\mu})_\nu=\frac{(2\zeta_1)^{5/2}(2\zeta_2)^{7/2}}{\sqrt{3}}\sum_{l=0,2}i^l\left\{3\zeta_1^2\,W_{3,3}^{l,\left(\frac{4-l}{2}\right)}-W_{3,3}^{l,\left(\frac{6-l}{2}\right)}\right\}\cdot O_l\left(\frac{R_\mu R_\nu}{R^2}\right)$$

$$(F_{2p_\mu,2p_\nu})_\sigma=2(4\zeta_1\zeta_2)^{7/2}\,i\sum_{l=1,3}i^l\,W_{3,3}^{l,\left(\frac{5-l}{2}\right)}\,O_l\left(\frac{R_\mu R_\nu R_\sigma}{R^3}\right)$$

Table 4. Integrals involving the dipole moment operator

$$(G_{n'n})_\mu \equiv \int d^3x\, \chi_{n'}(x - X_{j'})\,(x - X_j)_\mu\, \chi_n(x - X_j)$$

$$(G_{1s,1s})_\mu = 2(4\zeta_1\zeta_2)^{5/2}\, W_{2,3}^{1,1}\, \frac{R_\mu}{R}$$

$$(G_{1s,2s})_\mu = \frac{2(4\zeta_1\zeta_2)^{5/2}}{\sqrt{3}} (5\zeta_2^2\, W_{2,4}^{1,1} - W_{2,4}^{1,2})\, \frac{R_\mu}{R}$$

$$(G_{2s,2s})_\mu = \frac{2(4\zeta_1\zeta_2)^{5/2}}{3} \{15\zeta_1^2\zeta_2^2\, W_{3,4}^{1,1} - (3\zeta_1^2 + 5\zeta_2^2)\, W_{3,4}^{1,2} + W_{3,4}^{1,3}\}\, \frac{R_\mu}{R}$$

$$(G_{2p_\mu,1s})_\nu = 4(2\zeta_1)^{7/2}(2\zeta_2)^{5/2} \sum_{l=0,2} i^l\, W_{3,3}^{l,\left(\frac{4-l}{2}\right)}\, O_l\!\left(\frac{R_\mu R_\nu}{R^2}\right)$$

$$(G_{2p_\mu,2s})_\nu = \frac{4(2\zeta_1)^{7/2}(2\zeta_2)^{5/2}}{\sqrt{3}} \sum_{l=0,2} i^l \left\{5\zeta_2^2\, W_{3,4}^{l,\left(\frac{4-l}{2}\right)} - W_{3,4}^{l,\left(\frac{6-l}{2}\right)}\right\} O_l\!\left(\frac{R_\mu R_\nu}{R^2}\right)$$

$$(G_{2p_\mu,2p_\nu})_\sigma = -12(4\zeta_1\zeta_2)^{7/2} \left\{ i \sum_{l=1,3} i^l\, W_{3,4}^{l,\left(\frac{5-l}{2}\right)}\, O_l\!\left(\frac{R_\mu R_\nu R_\sigma}{R^3}\right) + \frac{1}{6}\, W_{3,3}^{1,1}\, \frac{R_\mu}{R}\, \delta_{\nu\sigma} \right\}$$

Table 5. Overlap integrals

$$S_{n'n} \equiv \int d^3x\, \chi_{n'}(x - X_{j'})\, \chi_n(x - X_j)$$

$$S_{1s,1s} = \tfrac{1}{2}(4\zeta_1\zeta_2)^{5/2}\, W_{2,2}^{0,1}$$

$$S_{1s,2p_\mu} = (2\zeta_1)^{5/2}(2\zeta_2)^{7/2}\, W_{2,3}^{1,1}\, \frac{R_\mu}{R}$$

$$S_{1s,2s} = \frac{(4\zeta_1\zeta_2)^{5/2}}{2\sqrt{3}} (3\zeta_2^2\, W_{2,3}^{0,1} - W_{2,3}^{0,2})$$

$$S_{2s,2s} = \frac{(4\zeta_1\zeta_2)^{5/2}}{6} \{9\zeta_1^2\zeta_2^2\, W_{3,3}^{0,1} - 3(\zeta_1^2 + \zeta_2^2)\, W_{3,3}^{0,2} + W_{3,3}^{0,3}\}$$

$$S_{2s,2p_\mu} = \frac{(2\zeta_1)^{5/2}(2\zeta_2)^{7/2}}{\sqrt{3}} (3\zeta_1^2\, W_{3,3}^{1,1} - W_{3,3}^{1,2})\, \frac{R_\mu}{R}$$

$$S_{2p_\mu,2p_\nu} = 2(4\zeta_1\zeta_2)^{7/2} \sum_{l=0,2} i^l\, W_{3,3}^{l,\left(\frac{4-l}{2}\right)}\, O_l\!\left(\frac{R_\mu R_\nu}{R^2}\right)$$

angular functions of Table 2 and the radial functions of Harris' Eq. (38), are given in Tables 3–8. For the sake of completeness, we have included all of the two-center one-electron integrals which are of interest for the calculation of optical properties of molecules. These include matrix elements of the momentum operator, the dipole operator, the tensor operator $x_\mu \frac{\partial}{\partial x_\nu}$, the quadrupole moment operator, and the angular momentum operator, and overlap integrals. The matrix elements were evaluated for Slater-type atomic orbitals up to $n = 2$. Applications will be reported in another paper.

Table 6. Integrals involving the operator $x_\mu \frac{\partial}{\partial x_\nu}$

$$(T_{n'n})_{\mu\nu} \equiv \int d^3x\, \chi_{n'}(\boldsymbol{x}-\boldsymbol{X}_{j'})\,(\boldsymbol{x}-\boldsymbol{X}_{j'})_\mu \frac{\partial}{\partial x_\nu} \chi_n(\boldsymbol{x}-\boldsymbol{X}_j)$$

$$(T_{1s,1s})_{\mu\nu} = -2(4\zeta_1\zeta_2)^{5/2} \sum_{l=0,2} i^l W_{3,2}^{l,\left(\frac{4-l}{2}\right)} O_l\left(\frac{R_\mu R_\nu}{R^2}\right)$$

$$(T_{1s,2s})_{\mu\nu} = -\frac{2}{\sqrt{3}}(4\zeta_1\zeta_2)^{5/2} \sum_{l=0,2} i^l \{3\zeta_2^2 W_{3,3}^{l,\left(\frac{4-l}{2}\right)} - W_{3,3}^{l,\left(\frac{6-l}{2}\right)}\} O_l\left(\frac{R_\mu R_\nu}{R^2}\right)$$

$$(T_{2s,2s})_{\mu\nu} = -\frac{2}{3}(4\zeta_1\zeta_2)^{5/2} \sum_{l=0,2} i^l \{15\zeta_1^2\zeta_2^2 W_{4,3}^{l,\left(\frac{4-l}{2}\right)} - (5\zeta_1^2+3\zeta_2^2)\, W_{4,3}^{l,\left(\frac{6-l}{2}\right)} + W_{4,3}^{l,\left(\frac{8-l}{2}\right)}\} O_l\left(\frac{R_\mu R_\nu}{R^2}\right)$$

$$(T_{1s,2p_\mu})_{\nu\sigma} = 4(2\zeta_1)^{5/2}(2\zeta_2)^{7/2}\, i \sum_{l=1,3} i^l W_{3,3}^{l,\left(\frac{5-l}{2}\right)} O_l\left(\frac{R_\mu R_\nu R_\sigma}{R^3}\right)$$

$$(T_{2s,2p_\mu})_{\nu\sigma} = \frac{4}{\sqrt{3}}(2\zeta_1)^{5/2}(2\zeta_2)^{7/2}\, i \sum_{l=1,3} i^l \cdot \left\{5\zeta_1^2 W_{4,3}^{l,\left(\frac{5-l}{2}\right)} - W_{4,3}^{l,\left(\frac{7-l}{2}\right)}\right\} O_l\left(\frac{R_\mu R_\nu R_\sigma}{R^3}\right)$$

$$(T_{2p_\mu,2p_\nu})_{\sigma\varrho} = 2(4\zeta_1\zeta_2)^{7/2}\left[\delta_{\mu\sigma} \sum_{l=0,2} i^l W_{3,3}^{l,\left(\frac{4-l}{2}\right)} O_l\left(\frac{R_\varrho R_\nu}{R^2}\right) - 6 \sum_{l=0,2,4} i^l W_{4,3}^{l,\left(\frac{6-l}{2}\right)} O_l\left(\frac{R_\mu R_\nu R_\sigma R_\varrho}{R^4}\right)\right]$$

Table 7. Integrals involving the quadrupole moment operator

$$(Q_{n'n})_{\mu\nu} \equiv \int d^3x\, \chi_{n'}(\boldsymbol{x}-\boldsymbol{X}_{j'})\,(\boldsymbol{x}-\boldsymbol{X}_{j'})_\mu\,(\boldsymbol{x}-\boldsymbol{X}_j)_\nu\, \chi_n(\boldsymbol{x}-\boldsymbol{X}_j)$$

$$(Q_{1s,1s})_{\mu\nu} = 8(4\zeta_1\zeta_2)^{5/2} \sum_{l=0,2} i^l W_{3,3}^{l,\left(\frac{4-l}{2}\right)} O_l\left(\frac{R_\mu R_\nu}{R^2}\right)$$

$$(Q_{1s,2s})_{\mu\nu} = \frac{8}{\sqrt{3}}(4\zeta_1\zeta_2)^{5/2} \sum_{l=0,2} i^l \{5\zeta_2^2 W_{3,4}^{l,\left(\frac{4-l}{2}\right)} - W_{3,4}^{l,\left(\frac{6-l}{2}\right)}\} O_l\left(\frac{R_\mu R_\nu}{R^2}\right)$$

$$(Q_{2s,2s})_{\mu\nu} = \frac{8}{3}(4\zeta_1\zeta_2)^{5/2} \sum_{l=0,2} i^l \left\{25\zeta_1^2\zeta_2^2 W_{4,4}^{l,\left(\frac{4-l}{2}\right)} - 5(\zeta_1^2+\zeta_2^2)\, W_{4,4}^{l,\left(\frac{6-l}{2}\right)} + W_{4,4}^{l,\left(\frac{8-l}{2}\right)}\right\} O_l\left(\frac{R_\mu R_\nu}{R^2}\right)$$

$$(Q_{1s,2p_\mu})_{\nu\sigma} = -4(2\zeta_1)^{5/2}(2\zeta_2)^{7/2}\left[\delta_{\mu\sigma} W_{3,3}^{1,1} \frac{R_\nu}{R} - 6 \sum_{l=1,3} i^{l-1} W_{3,4}^{l,\left(\frac{5-l}{2}\right)} O_l\left(\frac{R_\mu R_\nu R_\sigma}{R^3}\right)\right]$$

$$(Q_{2s,2p_\mu})_{\nu\sigma} = \frac{-4}{\sqrt{3}}(2\zeta_1)^{5/2}(2\zeta_2)^{7/2}\left[\delta_{\mu\sigma} \frac{R_\nu}{R}(5\zeta_1^2 W_{4,3}^{1,1} - W_{4,3}^{1,2}) - 6 \sum_{l=1,3} i^{l-1}\left\{5\zeta_1^2 W_{4,4}^{l,\left(\frac{5-l}{2}\right)} - W_{4,4}^{l,\left(\frac{7-l}{2}\right)}\right\} O_l\left(\frac{R_\mu R_\nu R_\sigma}{R^3}\right)\right]$$

$$(Q_{2p_\mu,2p_\nu})_{\sigma\varrho} = 2(4\zeta_1\zeta_2)^{7/2}\left[\delta_{\mu\sigma}\delta_{\nu\varrho} W_{3,3}^{0,1} - 6 \sum_{l=0,2} i^l \left\{\delta_{\mu\sigma} W_{3,4}^{l,\left(\frac{4-l}{2}\right)} \cdot O_l\left(\frac{R_\nu R_\varrho}{R^2}\right) + \delta_{\nu\varrho} W_{4,3}^{l,\left(\frac{4-l}{2}\right)} O_l\left(\frac{R_\mu R_\sigma}{R^2}\right)\right\} + 36 \sum_{l=0,2,4} i^l W_{4,4}^{l,\left(\frac{6-l}{2}\right)} O_l\left(\frac{R_\mu R_\nu R_\sigma R_\varrho}{R^4}\right)\right]$$

Table 8. Matrix elements of the angular momentum operator

$$(L_{n'n})_{\sigma\varrho} \equiv \int d^3x \chi_{n'}(\boldsymbol{x} - \boldsymbol{X}_{j'}) \left(x_\sigma \frac{\partial}{\partial x_\varrho} - x_\varrho \frac{\partial}{\partial x_\sigma} \right) \chi_n(\boldsymbol{x} - \boldsymbol{X}_j)$$

$$(L_{n's,ns})_{\sigma\varrho} = X_j^\sigma (F_{n's,ns})_\varrho - X_j^\varrho (F_{n's,ns})_\sigma$$

$$(L_{n's,2p_\mu})_{\sigma\varrho} = X_j^\sigma (F_{n's,2p_\mu})_\varrho - X_j^\varrho (F_{n's,2p_\mu})_\sigma$$

$$(L_{2p_\mu,2p_\nu})_{\sigma\varrho} = X_j^\sigma (F_{2p_\mu,2p_\nu})_\varrho - X_j^\varrho (F_{2p_\mu,2p_\nu})_\sigma + \delta_{\varrho\nu} S_{2p_\mu,2p_\nu} - \delta_{\sigma\nu} S_{2p_\mu,2p_\varrho}$$

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