

Analytic expressions for one-centre p -space integrals over Slater functions

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Analytic expressions for the assessment of orbital and total momentum values of atoms using Slater-type orbitals (STO) are formulated. A detailed description of the use of these expressions is reported. In order to test these expressions, we have carried out calculations of momentum expectation values and made comparisons with results based on numerical quadrature. These formulae are likely to be both more convenient and much more accurate.

1. Introduction

During the past years interest in Compton scattering as a tool for studying electronic momentum distributions in atoms, molecules and solids has increased [1,2]. The possibility of obtaining atomic and molecular total energies makes Compton scattering an extremely attractive technique, particularly since these energies are generally obtained from spectroscopic and thermodynamic quantities which are often difficult or impossible to be accurately measured.

Several theoretical studies of electron momentum distributions have been reported. Weiss et al. [3] computed the nonrelativistic Hartree–Fock Compton profiles of elements employing the double-zeta wave functions of Clementi [4]. Biggs et al. [5] calculated both relativistic and nonrelativistic Compton profiles for all free atoms up to $Z = 102$ employing numerical Hartree–Fock wave functions [6,7]. Ponce has tabulated orbital momentum expectation values for $\langle p \rangle$ and $\langle p^2 \rangle$ using Clementi and Roetti functions [9]. Nonrelativistic $\langle p^t \rangle$ values for $t = -2$ to 4 using the analytic Roothaan–Hartree–Fock atomic wave functions of Clementi and Roetti [9], for the ground and certain excited states of helium through xenon atoms and their singly charged positive and negative ions, have been tabulated by Gadre et al. [10]. Westgate et al. [11] have collected some total momentum expectation values and other momentum space properties for nonrelativistic functions [9,12]. All the mentioned evaluations of $\langle p^t \rangle$ values have been carried out using the electron momentum density by numerical quadrature. Some operators are directly

available from $\langle p' \rangle$: the Compton profile $J(0)$ is equal to $\langle p^{-1} \rangle / 2$, the Slater–Dirac exchange energy is proportional to $\langle p \rangle$, the electronic energy is equal to $\langle p^2 \rangle / 2$, the initial value of the Patterson function in X-ray crystallography is proportional to $\langle p^3 \rangle$, and relativistic corrections are proportional to $\langle p^4 \rangle$.

The analytical expressions for electron momentum distributions in the configurational Slater-type orbital approximation have been obtained for small atoms as well as for particular cases (only analytical formulae of 1s or 3d STO functions have been developed [13–16]). The aim of the present work is to describe formulae corresponding to orbital momentum values of STO functions.

2. Theory

Under the LCAO approximation an orbital function Φ_j is expressed as a linear combination of a noncomplete basis set $\{\varphi_i\}_{i=1}^n$:

$$\Phi_j(r) = \sum_{i=1}^n \varphi_i(r) c_{ij}. \quad (1)$$

The Fourier transform of this orbital is expressed either by the integral [17],

$$\hat{\Phi}_j(p) = (2\pi)^{-3/2} \int e^{-ipr} \Phi_j(r) dr, \quad (2)$$

where p is the momentum coordinate, or by a linear combination of the Fourier transforms of the basis set functions

$$\hat{\Phi}_j(p) = \sum_{i=1}^n \hat{\varphi}_i(p) c_{ij}. \quad (3)$$

For calculating orbital momentum expectation values $\langle p' \rangle$, eq. (3) will be employed. They are given by

$$\langle p' \rangle_j = \langle \hat{\Phi}_j | p' | \hat{\Phi}_j \rangle \quad (4)$$

and using the expansion of $\hat{\Phi}_j$ in the basis set

$$\langle p' \rangle_j = \sum_{i,m=1}^n c_{ij} c_{mj} \langle \hat{\varphi}_i | p' | \hat{\varphi}_m \rangle. \quad (5)$$

The matrix elements $\langle \hat{\varphi}_i | p' | \hat{\varphi}_m \rangle$ will be neglected when two functions with different quantum numbers l or m_l are involved in the integral. This is due to the angular dependence of $\hat{\varphi}(p)$, which in atomic problems is identical to that of the original $\varphi(r)$.

The momentum expectation values $\langle p' \rangle$ for the atom would be given by the addition of $\langle p' \rangle_j$ over all the spin orbitals N needed to describe the electronic atomic state,

Table 1
Normalization constants for Fourier transforms of STO functions.

	$l = 0$	$l = 1$	$l = 2$
$n = 1$	$(2\zeta_{1s}/\pi)^{1/2} 4\zeta_{1s}^2$		
$n = 2$	$(2\zeta_{2s}/3\pi)^{1/2} 4\zeta_{2s}^2$	$(2\zeta_{2p}/3\pi)^{1/2} 16\zeta_{2p}^3$	
$n = 3$	$(\zeta_{3s}/5\pi)^{1/2} 32\zeta_{3s}^4$	$(\zeta_{3s}/45\pi)^{1/2} 32\zeta_{3p}^3$	$(\zeta_{3d}/5\pi)^{1/2} 64\zeta_{3d}^4$
$n = 4$	$(2\zeta_{4s}/35\pi)^{1/2} 16\zeta_{4s}^4$	$(2\zeta_{4p}/35\pi)^{1/2} 32\zeta_{4p}^5$	$(2\zeta_{4d}/35\pi)^{1/2} 32\zeta_{4d}^4$
$n = 5$	$(\zeta_{5s}/63\pi)^{1/2} 64\zeta_{5s}^6$	$(\zeta_{5p}/1575\pi)^{1/2} 64\zeta_{5p}^5$	

$$\langle p^l \rangle = \sum_{j=1}^N \langle p^l \rangle_j. \tag{6}$$

From Fourier transforms of STOs given by Kaijser and Smith [18] the elements $\langle \hat{\varphi}_i | p^l | \hat{\varphi}_m \rangle$ can be calculated analytically. These transforms do not follow a generic formula capable of being integrated over p . However, all of them are a linear combination of positive powers of p and negative powers of $(\zeta_i^2 + p^2)$; this can be written as

$$\hat{\varphi}_i = -(i)^{l_i} (-1)^{l_i+1} N(\zeta_i) (p^2 + \zeta_i^2)^{-(n_i+1)} \sum_{k=0,2,4} F_k(\zeta_i) p^{k+l_i}, \tag{7}$$

where the normalization constant $N(\zeta_i)$, given in table 1 are powers of ζ_i multiplied by integer numbers, l_i and n_i are respectively the azimuthal and the principal quantum numbers of the φ_i function, ζ_i is the exponent, p the momentum variable and $F_k(\zeta_i)$ a factor constant in the integration over p coordinates, depending on ζ_i and k . The index k takes values 0, 2 or 4, not higher than 4 for $n_i + l_i \leq 6$, depending on the number of summands involved in the considered Fourier transform, $\hat{\varphi}_i$. These factors are summarized in table 2, where every row gives the factor for one basis function.

Table 2
Factors for Fourier transforms of STO functions.

	F_0	F_2	F_4
$\hat{\varphi}_{1s}$	1		
$\hat{\varphi}_{2s}$	$3\zeta_{2s}^2$	-1	
$\hat{\varphi}_{3s}$	ζ_{3s}^2	-1	
$\hat{\varphi}_{4s}$	$5\zeta_{4s}^4$	$-10\zeta_{4s}^2$	1
$\hat{\varphi}_{5s}$	$3\zeta_{5s}^4$	$-10\zeta_{5s}^2$	3
$\hat{\varphi}_{2p}$	1		
$\hat{\varphi}_{3p}$	$5\zeta_{3p}^2$	-1	
$\hat{\varphi}_{4p}$	$5\zeta_{4p}^4$	-3	
$\hat{\varphi}_{5p}$	$35\zeta_{5p}^4$	$-42\zeta_{5p}^2$	3
$\hat{\varphi}_{3d}$	1		
$\hat{\varphi}_{4d}$	$7\zeta_{4d}^2$	-1	

The number of summands required to calculate $\langle \hat{\varphi}_i | p^t | \hat{\varphi}_m \rangle$ depends on the number of summands involved in φ_i and φ_m Fourier transforms. Using eq. (7) for $\hat{\varphi}_i$ and $\hat{\varphi}_m$, those elements have the expression

$$\langle \hat{\varphi}_i | p^t | \hat{\varphi}_m \rangle = N(\zeta_i) N(\zeta_m) \sum_{k=0,2,4} \sum_{q=0,2,4} F_k(\zeta_i) F_q(\zeta_m) \int_0^\infty p^{k+q+l_i+l_m+2+t} (p^2 + \zeta_i^2)^{-(n_i+1)} (p^2 + \zeta_m^2)^{-(n_m+1)} dp. \quad (8)$$

Defining the new indices $\nu = (k + q + l_i + l_m + 3 + t)/2$, $\mu = n_i + 1$ and $\rho = n_m + 1$, the above integral is redesignated as $I(\zeta_i, \zeta_m, \nu, \mu, \rho)$,

$$\langle \hat{\varphi}_i | p^t | \hat{\varphi}_m \rangle = N(\zeta_i) N(\zeta_m) \sum_{k=0,2,4} \sum_{q=0,2,4} F_k(\zeta_i) F_q(\zeta_m) I(\zeta_i, \zeta_m, \nu, \mu, \rho). \quad (9)$$

These integrals can be solved with a variable change [19] and the solution is

$$I(\zeta_i, \zeta_m, \nu, \mu, \rho) = \frac{1}{2} \zeta_i^{-2\nu} \zeta_m^{2(\nu-\rho)} B(\nu, \mu - \nu + \rho) {}_2F_1(\mu, \nu; \mu + \rho; 1 - \zeta_m^2/\zeta_i^2) \quad (10)$$

when $\nu > 0$ and $\mu > (\nu - \rho)$ and where $B(a, b)$ is a beta function, defined by

$$B(a, b) = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)} \quad (11)$$

and ${}_2F_1$ is a hypergeometric function:

$${}_2F_1(a, b; c; z) = \sum_{k=0} \frac{(a)_k (b)_k z^k}{(c)_k k!} \quad (12)$$

with

$$(a)_k = a(a+1)(a+2) \dots (a+k-1). \quad (13)$$

Maximum and minimum p powers are given by the restriction required in eq. (10),

$$-(k + q + l_i + l_m + 3) < t < 2(n_i + n_m) - (l_i + l_m + k + q) + 1. \quad (14)$$

For example, for two 1s functions where $k = q = 0$, $l_i = l_m = 0$ and $n_i = n_m = 1$, the limits of the integral are $-3 < t < 5$. Explicit expressions of eq. (9), for 1s to 4d orbitals, are given in the appendix. These formulae are given as a function of normalization constants $N(\zeta_i)$, $N(\zeta_m)$ (see table 1), the exponents, ζ_i , ζ_m and the integrals $I(\zeta_i, \zeta_m, \nu, \mu, \rho)$. Notice that in the appendix, we have simplified the notation of the integrals of eq. (10), eliminating the two exponents involved in the calculated term.

3. Results and discussion

The atomic momentum expectation values ($Z \leq 54$) using any STO basis set can be investigated from the expressions in the appendix. These expressions make

Table 3

Orbital momentum expectation values $\langle p^1 \rangle$ and $\langle p^2 \rangle$ for the Mn (6S) atom.

	$\langle p^1 \rangle$		$\langle p^2 \rangle$	
	Ponce ^{a)}	This work	Ponce ^{a)}	This work
1s	0.2074285(+2)	0.207440(+2)	0.60091613(+3)	0.601488(+3)
2s	0.685909(+1)	0.685914(+1)	0.11006106(+3)	0.110112(+3)
2p	0.925438(+1)	0.925427(+1)	0.10748722(+3)	0.107486(+3)
3s	0.274873(+1)	0.274876(+1)	0.2270143(+2)	0.227085(+2)
3p	0.316308(+1)	0.316312(+1)	0.1973988(+2)	0.197404(+2)
3d	0.314002(+1)	0.314001(+1)	0.1294302(+2)	0.129430(+2)
4s	0.58296	0.583262	0.151329(+3)	0.151336(+1)

^{a)} From ref. [8].

possible to evaluate the $\langle p^t \rangle$ analytically. Numerical tests are carried out in this section to study the accuracy of the orbital and total momentum values obtained by using the Hartree–Fock limit function [9] of the Mn atom in the 6S state. All calculations are given in atomic units (for $\langle p^t \rangle \hbar^t a_0^{-t}$).

Table 3 summarizes orbital momentum expectation values obtained by Ponce and in this work. In the formulae proposed in this work, the number of significant figures for $\langle p^t \rangle$ is limited by the accuracy of the wave function. An ordering of the exponents, $\zeta_m \leq \zeta_i$, avoids the nonconvergence of the hypergeometrical series. Clementi wave functions [9] are tabulated with 6 digits but the significant figures of the coefficients change from 1 to 5. In order to give $\langle p^t \rangle$ values with 6 significant figures we have recalculated the orbital coefficients. A variation of between 4 and 6 figures is shown by comparing the orbital values of Ponce and the ones obtained with analytic formulae. The highest discrepancy is given for $\langle p \rangle_{4s}$ and $\langle p^2 \rangle_{1s}$.

Comparisons of $\langle p^t \rangle$ total values are shown in table 4. Here we compare our results with those of Gadre for $t = -2$ to 4 and with those of Ponce's for $t = 1$ and 2. The latter values have been calculated from the sum of corresponding orbital values given in table 3. The errors in $\langle p^t \rangle$ for our calculations are 10^{-6} , limited by

Table 4

Total momentum expectation values $\langle p^t \rangle$ for the Mn (6S) atom.

	Ponce ^{a)}	Gadre et al. ^{b)}	This work
-2		0.41195(+2)	0.411943(+2)
-1		0.14342(+2)	0.143422(+2)
1	0.15207212(+3)	0.15207(+3)	0.152075(+3)
2	0.229846152(+4)	0.22997(+4)	0.229971(+4)
3		0.70260(+5)	0.702606(+5)
4		0.44324(+7)	0.443241(+7)

^{a)} Calculated from orbital momentum expectation values of table 3.^{b)} From ref. [11].

the number of significant figures of the Hartree–Fock limit function used. As shown in both tables 3 and 4, the $\langle p^2 \rangle$ values by Ponce are those exhibiting the highest discrepancy when compared with ours. Differences with Gadre’s results are obtained in the 4th or 5th figures, both if Clementi’s coefficients [9] or recalculated coefficients (tables 3 and 4) are employed. The $\langle p' \rangle$ obtained from the proposed formulae have errors ten times smaller than Gadre’s values due to the numerical procedure used by those authors.

This study presents analytical formulae to obtain orbital and total momentum expectation values for STO functions. These values can be computed for $Z = 2$ to 54 and provide quick and accurate results for their atomic properties.

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Appendix

Analytic expressions for $\langle \hat{\varphi}_i | p' | \hat{\varphi}_m \rangle$ integrals with STO functions $1s, 2s, 3s, 4s, 5s, 2p, 3p, 4p, 5p, 3d$ and $4d$:

$$\langle \widehat{1s} | p' | \widehat{1s} \rangle = N_{1s} N_{1s} I \left(\frac{t+3}{2}, 2, 2 \right), \quad (\text{A.1})$$

$$\langle \widehat{1s} | p' | \widehat{2s} \rangle = N_{1s} N_{2s} \left[3\zeta_{2s}^2 I \left(\frac{t+3}{2}, 2, 3 \right) - I \left(\frac{t+5}{2}, 2, 3 \right) \right], \quad (\text{A.2})$$

$$\langle \widehat{1s} | p' | \widehat{3s} \rangle = N_{1s} N_{3s} \left[\zeta_{3s}^2 I \left(\frac{t+3}{2}, 2, 4 \right) - I \left(\frac{t+5}{2}, 2, 4 \right) \right], \quad (\text{A.3})$$

$$\begin{aligned} \langle \widehat{1s} | p' | \widehat{4s} \rangle = & N_{1s} N_{4s} \left[5\zeta_{4s}^4 I \left(\frac{t+3}{2}, 2, 5 \right) \right. \\ & \left. - 10\zeta_{4s}^2 I \left(\frac{t+5}{2}, 2, 5 \right) + I \left(\frac{t+7}{2}, 2, 5 \right) \right], \end{aligned} \quad (\text{A.4})$$

$$\begin{aligned} \langle \widehat{1s} | p' | \widehat{5s} \rangle = & N_{1s} N_{5s} \left[3\zeta_{4s}^4 I \left(\frac{t+3}{2}, 2, 6 \right) \right. \\ & \left. - 10\zeta_{5s}^2 I \left(\frac{t+5}{2}, 2, 6 \right) + 3I \left(\frac{t+7}{2}, 2, 6 \right) \right], \end{aligned} \quad (\text{A.5})$$

$$\begin{aligned} \langle \widehat{2s} | p' | \widehat{2s'} \rangle = & N_{2s} N_{2s'} \left[9 \zeta_{2s}^2 \zeta_{2s'}^2 I \left(\frac{t+3}{2}, 3, 3 \right) \right. \\ & \left. - 3(\zeta_{2s}^2 + \zeta_{2s'}^2) I \left(\frac{t+5}{2}, 3, 3 \right) + I \left(\frac{t+7}{2}, 3, 3 \right) \right], \end{aligned} \tag{A.6}$$

$$\begin{aligned} \langle \widehat{2s} | p' | \widehat{3s} \rangle = & N_{2s} N_{3s} \left[3 \zeta_{2s}^2 \zeta_{3s}^2 I \left(\frac{t+3}{2}, 3, 4 \right) \right. \\ & \left. - (3 \zeta_{2s}^2 + \zeta_{3s}^2) I \left(\frac{t+5}{2}, 3, 4 \right) + I \left(\frac{t+7}{2}, 3, 4 \right) \right], \end{aligned} \tag{A.7}$$

$$\begin{aligned} \langle \widehat{2s} | p' | \widehat{4s} \rangle = & N_{2s} N_{4s} \left[15 \zeta_{2s}^2 \zeta_{4s}^4 I \left(\frac{t+3}{2}, 3, 5 \right) \right. \\ & - 5(6 \zeta_{2s}^2 \zeta_{4s}^2 + \zeta_{4s}^4) I \left(\frac{t+5}{2}, 3, 5 \right) \\ & \left. + (3 \zeta_{2s}^2 + 10 \zeta_{4s}^2) I \left(\frac{t+7}{2}, 3, 5 \right) - I \left(\frac{t+9}{2}, 3, 5 \right) \right], \end{aligned} \tag{A.8}$$

$$\begin{aligned} \langle \widehat{2s} | p' | \widehat{5s} \rangle = & N_{2s} N_{5s} \left[9 \zeta_{2s}^2 \zeta_{5s}^4 I \left(\frac{t+3}{2}, 3, 6 \right) \right. \\ & - 3(10 \zeta_{2s}^2 \zeta_{5s}^4 + \zeta_{5s}^4) I \left(\frac{t+5}{2}, 3, 6 \right) \\ & \left. + (9 \zeta_{2s}^2 + 10 \zeta_{5s}^2) I \left(\frac{t+7}{2}, 3, 6 \right) - 3 I \left(\frac{t+9}{2}, 3, 6 \right) \right], \end{aligned} \tag{A.9}$$

$$\begin{aligned} \langle \widehat{3s} | p' | \widehat{3s'} \rangle = & N_{3s} N_{3s'} \left[\zeta_{3s}^2 \zeta_{3s'}^2 I \left(\frac{t+3}{2}, 4, 4 \right) \right. \\ & \left. - (\zeta_{3s}^2 + \zeta_{3s'}^2) I \left(\frac{t+5}{2}, 4, 4 \right) + I \left(\frac{t+7}{2}, 4, 4 \right) \right], \end{aligned} \tag{A.10}$$

$$\begin{aligned} \langle \widehat{3s} | p' | \widehat{4s} \rangle = & N_{3s} N_{4s} \left[5 \zeta_{4s}^4 \zeta_{3s}^2 I \left(\frac{t+3}{2}, 4, 5 \right) \right. \\ & - 5(2 \zeta_{4s}^2 \zeta_{3s}^2 + \zeta_{4s}^4) I \left(\frac{t+5}{2}, 4, 5 \right) \\ & \left. + (\zeta_{3s}^2 + 10 \zeta_{4s}^2) I \left(\frac{t+7}{2}, 4, 5 \right) - I \left(\frac{t+9}{2}, 4, 5 \right) \right], \end{aligned} \tag{A.11}$$

$$\begin{aligned}
\langle \widehat{3s} | p' | \widehat{5s} \rangle &= N_{3s} N_{5s} \left[3\zeta_{5s}^4 \zeta_{3s}^2 I\left(\frac{t+3}{2}, 4, 6\right) \right. \\
&\quad - (10\zeta_{5s}^2 \zeta_{3s}^2 + 3\zeta_{5s}^4) I\left(\frac{t+5}{2}, 4, 6\right) \\
&\quad \left. + (3\zeta_{3s}^2 + 10\zeta_{5s}^2) I\left(\frac{t+7}{2}, 4, 6\right) - 3I\left(\frac{t+9}{2}, 4, 6\right) \right], \quad (\text{A.12})
\end{aligned}$$

$$\begin{aligned}
\langle \widehat{4s} | p' | \widehat{4s'} \rangle &= N_{4s} N_{4s'} \left[25\zeta_{4s}^4 \zeta_{4s'}^4 I\left(\frac{t+3}{2}, 5, 5\right) \right. \\
&\quad - 50(\zeta_{4s}^4 \zeta_{4s'}^2 + \zeta_{4s}^2 \zeta_{4s'}^4) I\left(\frac{t+5}{2}, 5, 5\right) \\
&\quad + 5(\zeta_{4s}^4 + \zeta_{4s'}^4 + 20\zeta_{4s}^2 \zeta_{4s'}^2) I\left(\frac{t+7}{2}, 5, 5\right) \\
&\quad \left. - 10(\zeta_{4s}^2 + \zeta_{4s'}^2) I\left(\frac{t+9}{2}, 5, 5\right) + I\left(\frac{t+11}{2}, 5, 5\right) \right], \quad (\text{A.13})
\end{aligned}$$

$$\begin{aligned}
\langle \widehat{4s} | p' | \widehat{5s} \rangle &= N_{4s} N_{5s} \left[15\zeta_{5s}^4 \zeta_{4s}^4 I\left(\frac{t+3}{2}, 5, 6\right) \right. \\
&\quad - 10(5\zeta_{4s}^4 \zeta_{5s}^2 + 3\zeta_{5s}^4 \zeta_{4s}^2) I\left(\frac{t+5}{2}, 5, 6\right) \\
&\quad + (15\zeta_{4s}^4 + 3\zeta_{5s}^4 + 100\zeta_{4s}^2 \zeta_{5s}^2) I\left(\frac{t+7}{2}, 5, 6\right) \\
&\quad \left. - 10(3\zeta_{4s}^2 + \zeta_{5s}^2) I\left(\frac{t+9}{2}, 5, 6\right) + 3I\left(\frac{t+11}{2}, 5, 6\right) \right], \quad (\text{A.14})
\end{aligned}$$

$$\begin{aligned}
\langle \widehat{5s} | p' | \widehat{5s'} \rangle &= N_{5s} N_{5s'} \left[9\zeta_{5s}^4 \zeta_{5s'}^4 I\left(\frac{t+3}{2}, 6, 6\right) \right. \\
&\quad - 30(\zeta_{5s}^4 \zeta_{5s'}^2 + \zeta_{5s}^2 \zeta_{5s'}^4) I\left(\frac{t+5}{2}, 6, 6\right) \\
&\quad + (9\zeta_{5s}^4 + 9\zeta_{5s'}^4 + 100\zeta_{5s}^2 \zeta_{5s'}^2) I\left(\frac{t+7}{2}, 6, 6\right) \\
&\quad \left. - 30(\zeta_{5s}^2 + \zeta_{5s'}^2) I\left(\frac{t+9}{2}, 6, 6\right) + 9I\left(\frac{t+11}{2}, 6, 6\right) \right], \quad (\text{A.15})
\end{aligned}$$

$$\langle \widehat{2p} | p' | \widehat{2p}' \rangle = N_{2p} N_{2p'} I\left(\frac{t+5}{2}, 3, 3\right), \tag{A.16}$$

$$\langle \widehat{2p} | p' | \widehat{3p} \rangle = N_{2p} N_{3p} \left[5\zeta_{3p}^2 I\left(\frac{t+5}{2}, 3, 4\right) - I\left(\frac{t+7}{2}, 3, 4\right) \right], \tag{A.17}$$

$$\langle \widehat{2p} | p' | \widehat{4p} \rangle = N_{2p} N_{4p} \left[5\zeta_{4p}^2 I\left(\frac{t+5}{2}, 3, 5\right) - 3I\left(\frac{t+7}{2}, 3, 5\right) \right], \tag{A.18}$$

$$\begin{aligned} \langle \widehat{2p} | p' | \widehat{5p} \rangle = & N_{2p} N_{5p} \left[35\zeta_{5p}^4 I\left(\frac{t+5}{2}, 3, 6\right) - 42\zeta_{5p}^2 I\left(\frac{t+7}{2}, 3, 6\right) \right. \\ & \left. + 3I\left(\frac{t+9}{2}, 3, 6\right) \right], \end{aligned} \tag{A.19}$$

$$\begin{aligned} \langle \widehat{3p} | p' | \widehat{3p}' \rangle = & N_{3p} N_{3p'} \left[25\zeta_{3p}^2 \zeta_{3p'}^2 I\left(\frac{t+5}{2}, 4, 4\right) \right. \\ & \left. - 5(\zeta_{3p}^2 + \zeta_{3p'}^2) I\left(\frac{t+7}{2}, 4, 4\right) + I\left(\frac{t+9}{2}, 4, 4\right) \right], \end{aligned} \tag{A.20}$$

$$\begin{aligned} \langle \widehat{3p} | p' | \widehat{4p} \rangle = & N_{3p} N_{4p} \left[25\zeta_{3p}^2 \zeta_{4p}^2 I\left(\frac{t+5}{2}, 4, 5\right) \right. \\ & \left. - 5(3\zeta_{3p}^2 + \zeta_{4p}^2) I\left(\frac{t+7}{2}, 4, 5\right) + 3I\left(\frac{t+9}{2}, 4, 5\right) \right], \end{aligned} \tag{A.21}$$

$$\begin{aligned} \langle \widehat{3p} | p' | \widehat{5p} \rangle = & N_{3p} N_{5p} \left[175\zeta_{3p}^2 \zeta_{5p}^4 I\left(\frac{t+5}{2}, 4, 6\right) \right. \\ & - 35(6\zeta_{3p}^2 \zeta_{5p}^2 + \zeta_{5p}^4) I\left(\frac{t+7}{2}, 4, 6\right) \\ & \left. + 3(5\zeta_{3p}^2 + 14\zeta_{5p}^2) I\left(\frac{t+9}{2}, 4, 6\right) - 3I\left(\frac{t+11}{2}, 4, 6\right) \right], \end{aligned} \tag{A.22}$$

$$\begin{aligned} \langle \widehat{4p} | p' | \widehat{4p}' \rangle = & N_{4p} N_{4p'} \left[25\zeta_{4p}^2 \zeta_{4p'}^2 I\left(\frac{t+5}{2}, 5, 5\right) - 15(\zeta_{4p}^2 + \zeta_{4p'}^2) I\left(\frac{t+7}{2}, 5, 5\right) \right. \\ & \left. + 9I\left(\frac{t+9}{2}, 5, 5\right) \right], \end{aligned} \tag{A.23}$$

$$\begin{aligned} \langle \widehat{4p} | p' | \widehat{5p} \rangle = & N_{4p} N_{5p} \left[175 \zeta_{4p}^2 \zeta_{5p}^4 I \left(\frac{t+5}{2}, 5, 6 \right) \right. \\ & - 105 (2 \zeta_{4p}^2 \zeta_{5p}^2 + \zeta_{5p}^4) I \left(\frac{t+7}{2}, 5, 6 \right) \\ & \left. + 3 (5 \zeta_{4p}^2 + 42 \zeta_{5p}^2) I \left(\frac{t+9}{2}, 5, 6 \right) - 9 I \left(\frac{t+11}{2}, 5, 6 \right) \right], \quad (\text{A.24}) \end{aligned}$$

$$\begin{aligned} \langle \widehat{5p} | p' | \widehat{5p'} \rangle = & N_{5p} N_{5p'} \left[1225 \zeta_{5p}^4 \zeta_{5p'}^4 I \left(\frac{t+5}{2}, 6, 6 \right) \right. \\ & - 1470 (\zeta_{5p}^4 \zeta_{5p'}^2 + \zeta_{5p}^2 \zeta_{5p'}^4) I \left(\frac{t+7}{2}, 6, 6 \right) \\ & + 105 (\zeta_{5p}^4 + \zeta_{5p'}^4 + 1764 \zeta_{5p}^2 \zeta_{5p'}^2) I \left(\frac{t+9}{2}, 6, 6 \right) \\ & \left. - 126 (\zeta_{5p}^2 + \zeta_{5p'}^2) I \left(\frac{t+11}{2}, 6, 6 \right) + 9 I \left(\frac{t+13}{2}, 5, 5 \right) \right], \quad (\text{A.25}) \end{aligned}$$

$$\langle \widehat{3d} | p' | \widehat{3d'} \rangle = N_{3d} N_{3d'} I \left(\frac{t+7}{2}, 4, 4 \right), \quad (\text{A.26})$$

$$\langle \widehat{3d} | p' | \widehat{4d} \rangle = N_{3d} N_{4d} \left[7 \zeta_{4d}^2 I \left(\frac{t+7}{2}, 4, 5 \right) - I \left(\frac{t+9}{2}, 4, 5 \right) \right], \quad (\text{A.27})$$

$$\begin{aligned} \langle \widehat{4d} | p' | \widehat{4d'} \rangle = & N_{4d} N_{4d'} \left[49 \zeta_{4d}^2 \zeta_{4d'}^2 I \left(\frac{t+7}{2}, 5, 5 \right) \right. \\ & \left. - 7 (\zeta_{4d}^2 + \zeta_{4d'}^2) I \left(\frac{t+9}{2}, 5, 5 \right) + I \left(\frac{t+11}{2}, 5, 5 \right) \right]. \quad (\text{A.28}) \end{aligned}$$

References

- [1] W.A. Reed, *Acta Crystallogr. A* 32 (1976) 676.
- [2] B.G. Williams, *Compton Scattering: The Investigation of Electron Momentum Distributions* (McGraw Hill, New York, 1977).
- [3] R.J. Weiss, A. Harvey and W.C. Philips, *Philos. Mag.* 17 (1968) 241.
- [4] E. Clementi, *IBM J. Res. Dev.* 9 (1965) 2.
- [5] F. Biggs, L.B. Mendelsohn and J.B. Mann, *At. Data Nucl. Data Tables* 16 (1975) 201.
- [6] J.B. Mann, *At. Data Nucl. Data Tables* 12 (1973) 1.
- [7] J.B. Mann and J.T. Waber, *At. Data* 5 (1973) 201.
- [8] V.H. Ponce, *At. Data Nucl. Data Tables* 19 (1977) 63.

- [9] E. Clementi and C. Roetti, *At. Data Nucl. Data Tables* 14 (1974) 177.
- [10] S.R. Gadre, S.P. Gejji and S.J. Chakravorty, *At. Data Nucl. Data Tables* 28 (1983) 477.
- [11] W.M. Westgate, R.P. Sagar, A. Farazdei, V.H. Smith Jr., A.M. Simas and A.J. Thakkar, *At. Data Nucl. Data Tables* 48 (1991) 213.
- [12] A.D. McLean and R.S. McLean, *At. Data Nucl. Data Tables* 26 (1981) 197.
- [13] B. Tsapline, *C.R. Acad. Sci. Paris C274* (1971) 944.
- [14] I.R. Epstein, *Chem. Phys. Lett.* 9 (1971) 9.
- [15] F.F. Komarov and M.M. Temkin, *J. Phys. B* 9 (1976) L255.
- [16] A.J. Thakkar, A.M. Simas and V.H. Smith Jr., *Mol. Phys.* 41 (1980) 1153.
- [17] W.E. Duncanson and C.A. Coulson, *Proc. Phys. Soc.* 40 (1948) 175.
- [18] P. Kaijser and V.H. Smith Jr., *Adv. Quant. Chem.* 10 (1980) 37.
- [19] I.S. Gradshteyn and I.M. Ryzhik, *Table of Integrals, Series and Products* (Academic Press, San Diego, 1980) p. 286, eq. (3.197.1).