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Relativistic X-ray Elastic Scattering Factors for He–Ar from Dirac–Hartree–Fock Wave Functions

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Abstract

X-ray and electron elastic scattering factors for He through Ar ground states have been computed from Dirac–Hartree–Fock (DHF) wave functions. Differing from earlier studies, the present DHF wave functions are not restricted to single configurations and will go into the nonrelativistic Hartree–Fock (HF) ground states when the speed of light $c \to \infty$. The relativistic effects have been analyzed through the differences of scattering factors calculated at DHF and HF levels of theory. It has been found that the effects become stronger as the nuclear charge increases and anomalous behavior observed in the literature for C, N, O, Si, P and S is due to the use of either single- or average-energy multiconfiguration DHF wave functions to extract the relativistic effects for these systems preventing attainment of the correct nonrelativistic limit. Scattering factors of common ions of the first- and second-row elements and the valence state of C and Si are also given.

1. Introduction

Accurate prediction of atomic X-ray and electron scattering factors has been the topic of several recent theoretical studies (Thakkar & Smith, 1992; Wang, Sagar, Schmider & Smith, 1993; Rez, Rez & Grant, 1994; Su & Coppens, 1994; Wang, Esquivel, Smith & Bunge, 1995; Meyer, Müller & Schweig, 1995). Starting from the nonrelativistic Hartree–Fock (HF) scattering factors (Wang, Sagar, Schmider & Smith, 1993), relativistic interaction (Rez, Rez & Grant, 1994) and electron correlation (Wang, Esquivel, Smith & Bunge, 1995; Meyer, Müller & Schweig, 1995) are the two remaining large factors that have to be taken into account for accurate theoretical prediction. Meyer *et al.* (1995) have suggested that these two effects be considered in an additive manner and obtained the elastic scattering factors for He–Ar by including the relativistic correction to those calculated from configuration interaction (CI) wave functions. However, there are questions about the reliability of the relativistic effects they have used. They employed the relativistic scattering factors of Doyle & Turner (1968; see also Maslen, Fox & O'Keefe, 1992) to extract the relativistic effects. These relativistic scattering factors were obtained from the single-configuration Dirac–Hartree–Fock (DHF) wave functions of Coulthard (1967). We will show that these relativistic wave functions do not necessarily go into the nonrelativistic HF ground states when the speed of light $c \to \infty$; as a result, the obtained differences of scattering factors will not reflect genuine relativistic effects and to use them to correct the nonrelativistic CI scattering factors turns out to be inappropriate.

The early reported relativistic scattering factors have without exception been based on either single- or average-energy multiconfiguration DHF wave functions (Doyle & Turner, 1968; Su & Coppens, 1994; Rez, Rez & Grant, 1994), although general multiconfiguration programs have been available (Desclaux, 1975; Grant, McKenzie, Norrington, Mayers & Pyper, 1980; Rez, Rez & Grant, 1994). For closed-shell systems, the single-configuration ground-state DHF wave function will yield the nonrelativistic HF one when $c \to \infty$. However, this is not always true for open-shell systems. A conventional nonrelativistic HF wave function is made up of a single *L–S*-coupled configuration. In relativistic calculations, orbitals are described by quantum numbers $nljm_j$, thus the wave functions must be *jj* coupled. Therefore, a linear combination of several *jj*-coupled configurations may be required to approximate a pure *L–S* coupling, in which case a single-configuration DHF wave function has no direct relation to the *L–S*-coupled nonrelativistic HF ground state.

Furthermore, in order to arrive at the correct nonrelativistic limit and therefore be able to realistically display a *relativistic effect*, both the relativistic and nonrelativistic wave functions are required to be *jj* coupled, with the additional demand that radial parts for orbitals differing only in the total angular momentum quantum number j be allowed to vary independently from each other. This is standard practice in relativistic calculations but not in nonrelativistic ones, calling for a departure from conventional HF into *jj*-coupled HF, without which the correct nonrelativistic limit is not reached. Of course, to avoid a large energy penalty, these *jj*-coupled nonrelativistic HF wave functions must resemble single-configuration *L–S*-coupled HF, thus a multiconfigurational description is required. Therefore, it is appropriate to label the present treatment as a multiconfiguration DHF (MCDHF) and MCHF approach in contrast to the earlier single- or average-energy multiconfiguration DHF and HF treatments.

After the MCDHF wave functions of the ground-state atoms or ions are obtained, the X-ray scattering factors were evaluated through the Fourier transformation of the electron charge density, $\rho(r)$,

$$f_x(s) = 4\pi \int r^2\rho(r)[\sin(4\pi sr)/4\pi sr]\,\mathrm{d}r, \qquad (1)$$

where $s = \sin(\theta)/\lambda$ (Å^{-1}). Electron scattering factors for $s \neq 0$ can be obtained using the Mott formula,

$$f_{\mathrm{el}}(s) = 2\pi(me^2/h^2\varepsilon_0)[Z - f_x(s)]/(4\pi s)^2, \qquad (2)$$

where Z is the nuclear charge and ε_0 is the permittivity of vacuum. The above relation can be further simplified as

$$f_{\mathrm{el}}(s) = 0.023934[Z - f_x(s)]/s^2, \qquad (3)$$

where s is in Å^{-1} and $f_{\mathrm{el}}(s)$ is given in Å. For the $s = 0$ case, the electron scattering factor can be obtained through Ibers's relation (Ibers, 1958),

$$f_{\mathrm{el}}(0) = (\pi me^2/3h^2\varepsilon_0)\langle r^2\rangle = 0.529177\langle r^2\rangle/3, \qquad (4)$$

where $\langle r^2\rangle$ is the second-order radial moment in atomic units, a_0^2, and $f_{\mathrm{el}}(0)$ is given in Å. The Fourier transformation in (1) and the calculation of $\langle r^2\rangle$ in (4) have been carried out through the use of NAG routines (NAG, 1984) with the convergence threshold set to 10^{-8}.

In the following, we discuss briefly the MCDHF theory for atomic systems and then focus on the relativistic effects on X-ray scattering factors.

2. MCDHF treatment of He through Ar

Detailed accounts of the multiconfiguration DHF methodology have been discussed by Bunge, Jáuregui & Ley-Koo (1996) and we will mention only those that are pertinent to the present study. The one-particle basis used consists of Dirac bispinors

$$\Psi^{(i)}_{n_i ljm_j} = \frac{1}{r}\begin{pmatrix} P_{n_i lj}(r)\mathcal{Y}_{\kappa m_j} \\ iQ_{n_i l'j}(r)\mathcal{Y}_{-\kappa m_j} \end{pmatrix} \quad i = 1, 2, \ldots, i_x(lj), \qquad (5)$$

where the angular functions $\mathcal{Y}_{\kappa m_j}$ are expressed in terms of Clebsch–Gordan coefficients, normalized spherical harmonics and two-component Pauli spinors. The radial part of the upper component is expressed as linear combinations of Slater-type orbitals $S_{n_k lj}(r)$:

$$P_{n_i lj} = \sum_k S_{n_k lj}(r)a_{klji}, \qquad (6)$$

$$S_{n_k lj}(r) = r^{\gamma+n_k-1}\exp(-\lambda_k r), \qquad (7)$$

where $\gamma = [\kappa^2 - (\alpha Z)^2]^{1/2} \geq \frac{1}{2}$, *viz* $Z \leq 118$. Moreover, each lower component Q is coupled to the upper component P (Lee & McLean, 1982; Ishikawa, Binning & Sando, 1983) through the kinetic balance condition (Stanton & Havriliak, 1984).

$$Q(r) = (\alpha/2)(\mathrm{d}/\mathrm{d}r + \kappa/r)P(r). \qquad (8)$$

The only exceptions to the above are when $\kappa > 0$ and $n = l + 1$, *viz* for $2p_{1/2}$, $3d_{3/2}$, $4f_{5/2}$ *etc.*, and for $1s_{1/2}$ orbitals, where the P's and Q's become hydrogenic eigensolutions (Mizushima, 1970), that is, eigenfunctions of *Dirac*'s equation with arbitrary charge $Z = n\lambda$. It has been shown (Bunge, Jáuregui & Ley-Koo, 1996) that these bases yield strict upper bounds to the eigenvalues of the one-particle *Dirac* Hamiltonian and also that they are within the domain of the *Dirac–Coulomb* *N*-particle Hamiltonian. In this way, and using a recently developed theory (Jáuregui, Bunge & Ley-Koo, 1995) for the *N*-particle *Dirac* equation, we overcome the usual problems of 'continuum dissolution' and 'variational collapse' haunting relativistic *N*-electron calculations.

The *N*-electron DHF ground-state wave function may in general be expressed as a linear combination of configurations that are eigenfunctions of J^2 with eigenvalue $\hbar^2 J(J+1)$. Each configuration is in turn given as a sum of Slater determinants with coefficients determined by angular-momentum couplings. The calculation of DHF wave functions is centered on the finding of the best occupied orbitals and, in the case of multiconfiguration wave functions, the finding also of the expansion coefficients. We will address only the latter problem here. Note that the present calculations use a point nucleus and the speed of light $c = 137.0359895$ a.u. (bohr s^{-1}) (Cohen & Taylor, 1987).

By definition, the conventional *L–S*-coupled HF ground state is made up of a single configuration. When going to *jj* coupling, however, some of these *L–S* single configurations turn out to be linear combinations of *jj* configurations with fixed coefficients. Those that require more than one configuration are the C, N, O, Si, P and S ground states. The multiconfiguration representations for these systems are given as follows:

C, Si: p^2,

$$^3P = (1/3^{1/2})[2^{1/2}p^2 + P^2], \quad J = 0; \qquad (9)$$

Table 1. *Total atomic DHF, single-configuration DHF (SC-DHF), HF and jj-HF energies (in hartree) for He through Ar*

1 hartree = 2643.6 kJ mol^{-1}.

Element	J	DHF$^{(a)}$	SC-DHF$^{(b)}$	HF$^{(c)}$	*jj*-HF$^{(d)}$
He	0	−2.86181334	−2.86181335	−2.86168000	−2.86168000
Li$^+$	0	−7.23720552		−7.23641520	−7.23641520
Li	1/2	−7.43353328	−7.43353322	−7.43272692	−7.43272692
Be^{2+}	0	−13.61400141		−13.61129943	−13.61129943
Be	0	−14.57589223	−14.5758919	−14.57302313	−14.57302313
B	1/2	−24.53661778	−24.5366169	−24.52906072	−24.52906072
C(val.)	2	−37.61504089		−37.59921440	−37.59921440
C(1*c*)	0	−37.65741580	−37.6574196		
C	0	−37.70513447		−37.68861890	−37.68861890
N(1*c*)	3/2	−54.31695274	−54.3169626		
N	3/2	−54.43247077		−54.40093415	−54.40093415
O(1*c*)	2	−74.83933251	−74.8393234		
O	2	−74.86569470		−74.80939840	−74.80953133
F	3/2	−99.50232126	−99.5023027	−99.40934928	−99.40937101
F$^-$	0	−99.55128745		−99.45945316	−99.45945316
Ne	0	−128.69196931	−128.691938	−128.5470980	−128.5470980
Na$^+$	0	−161.89596807		−161.6769624	−161.6769624
Na	1/2	−162.0781499	−162.078100	−161.8589116	−161.8589116
Mg^{2+}	0	−199.15013724		−198.8308102	−198.8308102
Mg	0	−199.9351590	−199.935083	−199.6146363	−199.6146363
Al	1/2	−242.3312554	−242.331141	−241.8767072	−241.8767180
Si(val.)	2	−289.3880074		−288.7630393	−288.7630393
Si(1*c*)	0	−289.45002596	−289.449869		
Si	0	−289.4820010		−288.8543624	−288.8543626
P(1*c*)	3/2	−341.48915137	−341.488962		
P	3/2	−341.56483558		−340.7187808	−340.7187808
S(1*c*)	2	−389.6090530	−389.608749		
S	2	−398.6256700		−397.5048958	−397.5049596
Cl	3/2	−460.9403061	−460.939870	−459.4820721	−459.4820892
Cl$^-$	0	−461.0330557		−459.5769189	−459.5769189
Ar	0	−528.6844505	−528.683840	−526.8175126	−526.8175126

(*a*) Present calculation. (*b*) Mohanty & Clementi (1989) employing the multiconfiguration relativistic program of Grant *et al.* (1980). (*c*) Bunge *et al.* (1992, 1993). (*d*) Bunge *et al.* (1996).

N, P: p^3,

$$^4S = (1/3)[2^{1/2}p^2P + 5^{1/2}pP^2 + 2^{1/2}P^3], \quad J = 3/2; \qquad (10)$$

O, S: p^4,

$$^3P = (1/3^{1/2})[2^{1/2}p^2P^2 - pP^3], \quad J = 2; \qquad (11)$$

where lower and upper cases indicate $j = l - 1/2$ and $j = l + 1/2$, respectively, and the radial parts of p and P are assumed to be the same. Note that in the present MCDHF calculation the expansion coefficients of the configurations may be varied.

Besides using multiconfiguration DHF wave functions for C, N, O, Si, P and S, we have also taken only the first term from (9)–(11) to carry out single-configuration DHF calculations for these six systems, in order to gain insight into the early relativistic studies. In the limit $c \rightarrow \infty$, the multiconfiguration wave functions related to (9)–(11) yield the corresponding nonrelativistic HF solutions, and relativistic correlation energies go smoothly into their nonrelativistic counterparts. However, the single-configuration results do not share these properties.

3. Results and discussion

3.1. *Ground-state energies of He–Ar*

In Table 1, we compile the DHF and HF ground-state energies of neutral and commonly occurring charged ions from He to Ar. For systems where a single configuration is adequate, the present DHF energy agrees with the previous calculations (Grant, McKenzie, Norrington, Mayers & Pyper, 1980; Mohanty & Clementi, 1989) very well. The deviation may be largely due to the use of slightly different c; 137.0373 a.u. *vs* the present value of 137.0359895 a.u. (Cohen & Taylor, 1987). For those six elements that require multiconfiguration wave functions for their ground states, we have tabulated both the multi- and single-configuration DHF results. The single-configuration DHF energies, which are labeled (1*c*) in Table 1, also agree with the earlier treatments (Mohanty & Clementi, 1989). We conclude that these are indeed the single-configuration DHF wave functions that have been employed before to represent these open-shell systems. As expected, the present multiconfiguration DHF energies for C and N ground states are found to be lower than the corresponding HF values (Bunge, Barri-

Table 2. *X-ray elastic scattering factors of He–Ne from multiconfiguration DHF wave functions*

$\sin\theta/\lambda(\text{Å}^{-1})$	He	Li	Be	B	C	N	O	F	Ne
0.00	2.0000	3.0000	4.0000	5.0000	6.0000	7.0000	8.0000	9.0000	10.0000
0.01	1.9983	2.9864	3.9873	4.9884	5.9899	6.9911	7.9918	8.9925	9.9931
0.02	1.9930	2.9465	3.9497	4.9537	5.9596	6.9646	7.9673	8.9699	9.9725
0.03	1.9844	2.8836	3.8886	4.8971	5.9099	6.9207	7.9267	8.9326	9.9382
0.04	1.9724	2.8021	3.8066	4.8200	5.8415	6.8602	7.8706	8.8809	9.8907
0.05	1.9571	2.7075	3.7067	4.7244	5.7559	6.7838	7.7996	8.8152	9.8302
0.06	1.9387	2.6056	3.5924	4.6128	5.6544	6.6925	7.7143	8.7361	9.7571
0.07	1.9174	2.5016	3.4675	4.4878	5.5389	6.5876	7.6157	8.6443	9.6721
0.08	1.8932	2.3998	3.3357	4.3522	5.4111	6.4702	7.5049	8.5406	9.5757
0.09	1.8664	2.3035	3.2006	4.2086	5.2731	6.3417	7.3829	8.4259	9.4686
0.10	1.8372	2.2151	3.0653	4.0599	5.1269	6.2037	7.2508	8.3010	9.3515
0.11	1.8058	2.1355	2.9325	3.9084	4.9744	6.0576	7.1100	8.1669	9.2251
0.12	1.7724	2.0651	2.8044	3.7565	4.8174	5.9049	6.9614	8.0246	9.0903
0.13	1.7373	2.0035	2.6826	3.6061	4.6579	5.7469	6.8065	7.8752	8.9479
0.14	1.7006	1.9500	2.5685	3.4588	4.4973	5.5851	6.6463	7.7195	8.7986
0.15	1.6626	1.9036	2.4626	3.3160	4.3373	5.4209	6.4820	7.5586	8.6434
0.16	1.6236	1.8633	2.3653	3.1789	4.1789	5.2553	6.3147	7.3934	8.4829
0.17	1.5836	1.8278	2.2767	3.0481	4.0235	5.0897	6.1454	7.2249	8.3181
0.18	1.5429	1.7963	2.1966	2.9243	3.8720	4.9248	5.9752	7.0538	8.1497
0.19	1.5018	1.7678	2.1244	2.8079	3.7250	4.7618	5.8048	6.8811	7.9785
0.20	1.4604	1.7416	2.0598	2.6989	3.5833	4.6014	5.6351	6.7076	7.8050
0.22	1.3773	1.6935	1.9507	2.5033	3.3173	4.2909	5.3006	6.3606	7.4543
0.24	1.2948	1.6483	1.8641	2.3362	3.0762	3.9976	4.9765	6.0179	7.1026
0.25	1.2542	1.6260	1.8276	2.2627	2.9653	3.8584	4.8196	5.8495	6.9276
0.26	1.2140	1.6037	1.7950	2.1953	2.8607	3.7244	4.6666	5.6836	6.7539
0.28	1.1356	1.5587	1.7389	2.0773	2.6703	3.4728	4.3734	5.3609	6.4119
0.30	1.0602	1.5127	1.6923	1.9790	2.5034	3.2433	4.0986	5.0521	6.0793
0.32	0.9883	1.4655	1.6522	1.8972	2.3582	3.0356	3.8430	4.7591	5.7583
0.34	0.9200	1.4175	1.6164	1.8289	2.2325	2.8490	3.6069	4.4827	5.4506
0.35	0.8873	1.3932	1.5996	1.7989	2.1763	2.7632	3.4961	4.3510	5.3022
0.36	0.8556	1.3687	1.5832	1.7715	2.1242	2.6823	3.3901	4.2236	5.1574
0.38	0.7950	1.3196	1.5515	1.7227	2.0309	2.5340	3.1920	3.9820	4.8794
0.40	0.7384	1.2704	1.5205	1.6808	1.9507	2.4026	3.0118	3.7575	4.6170
0.42	0.6855	1.2214	1.4895	1.6440	1.8816	2.2864	2.8484	3.5499	4.3702
0.44	0.6363	1.1730	1.4584	1.6111	1.8220	2.1840	2.7007	3.3585	4.1391
0.45	0.6130	1.1490	1.4427	1.5958	1.7952	2.1375	2.6324	3.2686	4.0292
0.46	0.5906	1.1252	1.4268	1.5811	1.7701	2.0938	2.5675	3.1825	3.9231
0.48	0.5482	1.0784	1.3948	1.5531	1.7249	2.0144	2.4477	3.0210	3.7220
0.50	0.5089	1.0326	1.3623	1.5265	1.6850	1.9443	2.3400	2.8733	3.5350
0.55	0.4232	0.9236	1.2794	1.4634	1.6026	1.8029	2.1167	2.5579	3.1256
0.60	0.3529	0.8233	1.1953	1.4017	1.5363	1.6973	1.9465	2.3083	2.7899
0.65	0.2953	0.7323	1.1117	1.3393	1.4787	1.6159	1.8160	2.1115	2.5168
0.70	0.2481	0.6504	1.0299	1.2758	1.4253	1.5501	1.7146	1.9562	2.2954
0.80	0.1773	0.5124	0.8764	1.1472	1.3218	1.4441	1.5680	1.7345	1.9713
0.90	0.1289	0.4043	0.7399	1.0205	1.2180	1.3522	1.4631	1.5879	1.7566
1.00	0.0953	0.3202	0.6222	0.9004	1.1138	1.2640	1.3767	1.4823	1.6094
1.10	0.0716	0.2551	0.5223	0.7898	1.0115	1.1762	1.2976	1.3979	1.5021
1.20	0.0546	0.2046	0.4386	0.6902	0.9134	1.0889	1.2209	1.3237	1.4177
1.30	0.0422	0.1652	0.3688	0.6019	0.8212	1.0034	1.1451	1.2541	1.3458
1.40	0.0331	0.1343	0.3109	0.5243	0.7360	0.9207	1.0702	1.1866	1.2805
1.50	0.0262	0.1100	0.2629	0.4567	0.6582	0.8421	0.9968	1.1201	1.2185
1.60	0.0210	0.0907	0.2231	0.3981	0.5879	0.7682	0.9256	1.0546	1.1583
1.70	0.0170	0.0753	0.1900	0.3474	0.5247	0.6994	0.8572	0.9905	1.0993
1.80	0.0139	0.0629	0.1624	0.3036	0.4682	0.6358	0.7922	0.9280	1.0412
1.90	0.0114	0.0529	0.1394	0.2659	0.4179	0.5776	0.7308	0.8677	0.9843
2.00	0.0095	0.0447	0.1200	0.2333	0.3732	0.5243	0.6733	0.8099	0.9289
2.50	0.0042	0.0209	0.0602	0.1257	0.2157	0.3241	0.4430	0.5640	0.6804
3.00	0.0029	0.0109	0.0328	0.0718	0.1294	0.2041	0.2923	0.3891	0.4893
3.50	0.0012	0.0062	0.0192	0.0434	0.0809	0.1321	0.1961	0.2701	0.3511
4.00	0.0007	0.0037	0.0118	0.0275	0.0525	0.0881	0.1343	0.1901	0.2537
5.00	0.0003	0.0016	0.0052	0.0124	0.0245	0.0426	0.0674	0.0991	0.1374
6.00	0.0001	0.0008	0.0026	0.0063	0.0127	0.0227	0.0367	0.0553	0.0787

Table 3. *X-ray elastic scattering factors of Na–Ar from multiconfiguration DHF wave functions*

$\sin\theta/\lambda(\text{Å}^{-1})$	Na	Mg	Al	Si	P	S	Cl	Ar
0.00	11.0000	12.0000	13.0000	14.0000	15.0000	16.0000	17.0000	18.0000
0.01	10.9802	11.9783	12.9755	13.9764	14.9778	15.9786	16.9797	17.9809
0.02	10.9220	11.9144	12.9031	13.9062	14.9117	15.9148	16.9192	17.9238
0.03	10.8298	11.8112	12.7859	13.7919	14.8034	15.8099	16.8196	17.8296
0.04	10.7093	11.6735	12.6292	13.6370	14.6555	15.6662	16.6825	17.6997
0.05	10.5678	11.5073	12.4390	13.4463	14.4715	15.4865	16.5103	17.5358
0.06	10.4123	11.3191	12.2224	13.2253	14.2557	15.2744	16.3058	17.3402
0.07	10.2493	11.1156	11.9867	12.9801	14.0127	15.0336	16.0722	17.1157
0.08	10.0840	10.9032	11.7387	12.7165	13.7474	14.7686	15.8130	16.8650
0.09	9.9202	10.6872	11.4845	12.4407	13.4650	14.4837	15.5321	16.5913
0.10	9.7601	10.4724	11.2295	12.1579	13.1703	14.1833	15.2331	16.2978
0.11	9.6049	10.2620	10.9781	11.8730	12.8679	13.8717	14.9199	15.9879
0.12	9.4546	10.0587	10.7333	11.5904	12.5622	13.5530	14.5962	15.6647
0.13	9.3087	9.8639	10.4977	11.3133	12.2569	13.2309	14.2654	15.3315
0.14	9.1664	9.6783	10.2727	11.0445	11.9553	12.9088	13.9309	14.9914
0.15	9.0267	9.5019	10.0592	10.7859	11.6602	12.5896	13.5956	14.6472
0.16	8.8885	9.3343	9.8573	10.5390	11.3738	12.2759	13.2623	14.3015
0.17	8.7509	9.1748	9.6668	10.3045	11.0978	11.9698	12.9333	13.9568
0.18	8.6132	9.0225	9.4873	10.0828	10.8335	11.6730	12.6105	13.6152
0.19	8.4748	8.8764	9.3180	9.8739	10.5815	11.3869	12.2958	13.2787
0.20	8.3354	8.7355	9.1581	9.6774	10.3425	11.1124	11.9904	12.9488
0.22	8.0525	8.4653	8.8623	9.3192	9.9033	10.6005	11.4118	12.3145
0.24	7.7643	8.2054	8.5923	9.0022	9.5141	10.1394	10.8803	11.7205
0.25	7.6184	8.0777	8.4647	8.8569	9.3369	9.9276	10.6330	11.4402
0.26	7.4716	7.9508	8.3411	8.7193	9.1704	9.7278	10.3980	11.1717
0.28	7.1765	7.6985	8.1028	8.4634	8.8663	9.3624	9.9642	10.6702
0.30	6.8811	7.4466	7.8730	8.2280	8.5954	9.0384	9.5764	10.2158
0.32	6.5876	7.1947	7.6481	8.0078	8.3516	8.7505	9.2310	9.8067
0.34	6.2982	6.9427	7.4261	7.7981	8.1291	8.4931	8.9234	9.4402
0.35	6.1556	6.8169	7.3156	7.6961	8.0243	8.3743	8.7824	9.2717
0.36	6.0146	6.6914	7.2054	7.5955	7.9230	8.2612	8.6491	9.1125
0.38	5.7386	6.4416	6.9855	7.3975	7.7290	8.0500	8.4033	8.8197
0.40	5.4713	6.1945	6.7662	7.2022	7.5437	7.8550	8.1816	8.5576
0.42	5.2137	5.9511	6.5477	7.0085	7.3645	7.6728	7.9799	8.3223
0.44	4.9667	5.7125	6.3305	6.8157	7.1893	7.5002	7.7944	8.1098
0.45	4.8473	5.5952	6.2225	6.7195	7.1027	7.4167	7.7068	8.0110
0.46	4.7308	5.4795	6.1151	6.6235	7.0166	7.3347	7.6220	7.9166
0.48	4.5062	5.2530	5.9021	6.4319	6.8454	7.1743	7.4598	7.7394
0.50	4.2932	5.0336	5.6924	6.2411	6.6751	7.0174	7.3055	7.5753
0.55	3.8108	4.5196	5.1861	5.7702	6.2514	6.6335	6.9421	7.2068
0.60	3.3973	4.0585	4.7123	5.3137	5.8316	6.2545	6.5955	6.8749
0.65	3.0472	3.6514	4.2770	4.8786	5.4197	5.8779	6.2546	6.5601
0.70	2.7534	3.2965	3.8831	4.4709	5.0214	5.5057	5.9155	6.2519
0.80	2.3050	2.7282	3.2205	3.7509	4.2850	4.7901	5.2459	5.6393
0.90	1.9967	2.3164	2.7114	3.1643	3.6494	4.1382	4.6071	5.0355
1.00	1.7840	2.0220	2.3301	2.7021	3.1224	3.5699	4.0230	4.4597
1.10	1.6340	1.8118	2.0484	2.3462	2.6983	3.0915	3.5089	3.9309
1.20	1.5237	1.6596	1.8410	2.0758	2.3640	2.6991	3.0701	3.4613
1.30	1.4380	1.5464	1.6873	1.8715	2.1039	2.3834	2.7043	3.0556
1.40	1.3668	1.4587	1.5713	1.7167	1.9027	2.1325	2.4046	2.7124
1.50	1.3041	1.3872	1.4811	1.5979	1.7472	1.9346	2.1620	2.4267
1.60	1.2462	1.3258	1.4082	1.5049	1.6260	1.7787	1.9672	2.1918
1.70	1.1909	1.2704	1.3466	1.4300	1.5302	1.6554	1.8111	2.0000
1.80	1.1372	1.2187	1.2923	1.3674	1.4528	1.5568	1.6859	1.8441
1.90	1.0845	1.1690	1.2427	1.3131	1.3886	1.4769	1.5848	1.7174
2.00	1.0327	1.1207	1.1958	1.2645	1.3336	1.4107	1.5023	1.6139
2.50	0.7911	0.8916	0.9795	1.0556	1.1221	1.1825	1.2405	1.3007
3.00	0.5913	0.6905	0.7830	0.8671	0.9423	1.0091	1.0686	1.1227
3.50	0.4380	0.5270	0.6146	0.6986	0.7771	0.8495	0.9151	0.9743
4.00	0.3248	0.4006	0.4784	0.5562	0.6321	0.7047	0.7729	0.8362
5.00	0.1827	0.2340	0.2899	0.3492	0.4108	0.4735	0.5360	0.5974
6.00	0.1074	0.1411	0.1794	0.2218	0.2676	0.3162	0.3669	0.4187

Table 4. *X-ray elastic scattering factors of ions and valence state C and Si from multiconfiguration DHF wave functions*

$\sin\theta/\lambda$(Å^{-1})	Li$^+$	Be^{2+}	C(val.)	F$^-$	Na$^+$	Mg^{2+}	Si(val.)	Cl$^-$
0.00	2.0000	2.0000	6.0000	10.0000	10.0000	10.0000	14.0000	18.0000
0.01	1.9993	1.9997	5.9900	9.9882	9.9953	9.9965	13.9762	17.9718
0.02	1.9974	1.9986	5.9603	9.9532	9.9811	9.9861	13.9057	17.8879
0.03	1.9941	1.9969	5.9115	9.8954	9.9577	9.9688	13.7905	17.7505
0.04	1.9895	1.9945	5.8443	9.8158	9.9249	9.9447	13.6344	17.5632
0.05	1.9837	1.9915	5.7601	9.7158	9.8831	9.9138	13.4418	17.3304
0.06	1.9766	1.9878	5.6604	9.5968	9.8325	9.8763	13.2183	17.0576
0.07	1.9683	1.9834	5.5467	9.4606	9.7731	9.8322	12.9698	16.7506
0.08	1.9587	1.9783	5.4209	9.3090	9.7054	9.7817	12.7023	16.4155
0.09	1.9479	1.9726	5.2850	9.1439	9.6296	9.7250	12.4218	16.0584
0.10	1.9360	1.9663	5.1408	8.9673	9.5460	9.6622	12.1341	15.6851
0.11	1.9230	1.9593	4.9903	8.7810	9.4551	9.5936	11.8440	15.3010
0.12	1.9089	1.9517	4.8354	8.5868	9.3572	9.5194	11.5562	14.9110
0.13	1.8938	1.9436	4.6778	8.3864	9.2527	9.4397	11.2741	14.5195
0.14	1.8777	1.9348	4.5192	8.1814	9.1420	9.3548	11.0008	14.1304
0.15	1.8606	1.9254	4.3609	7.9731	9.0256	9.2651	10.7384	13.7467
0.16	1.8426	1.9155	4.2042	7.7630	8.9040	9.1706	10.4885	13.3712
0.17	1.8237	1.9050	4.0503	7.5521	8.7775	9.0717	10.2520	13.0059
0.18	1.8041	1.8939	3.9002	7.3415	8.6466	8.9688	10.0292	12.6526
0.19	1.7836	1.8824	3.7546	7.1321	8.5119	8.8619	9.8201	12.3125
0.20	1.7625	1.8703	3.6141	6.9248	8.3737	8.7515	9.6244	11.9865
0.22	1.7183	1.8448	3.3501	6.5187	8.0887	8.5212	9.2703	11.3789
0.24	1.6719	1.8174	3.1107	6.1276	7.7952	8.2800	8.9599	10.8313
0.25	1.6480	1.8031	3.0005	5.9386	7.6462	8.1561	8.8186	10.5797
0.26	1.6237	1.7884	2.8965	5.7544	7.4963	8.0302	8.6852	10.3422
0.28	1.5741	1.7578	2.7068	5.4012	7.1952	7.7741	8.4382	9.9080
0.30	1.5234	1.7259	2.5403	5.0691	6.8946	7.5136	8.2117	9.5238
0.32	1.4720	1.6928	2.3952	4.7585	6.5967	7.2508	7.9994	9.1842
0.34	1.4203	1.6586	2.2692	4.4695	6.3038	6.9874	7.7967	8.8835
0.35	1.3943	1.6411	2.2126	4.3329	6.1597	6.8560	7.6977	8.7460
0.36	1.3685	1.6235	2.1601	4.2015	6.0175	6.7251	7.5998	8.6163
0.38	1.3169	1.5876	2.0658	3.9540	5.7394	6.4655	7.4062	8.3773
0.40	1.2658	1.5511	1.9843	3.7261	5.4706	6.2098	7.2140	8.1617
0.42	1.2154	1.5142	1.9136	3.5168	5.2120	5.9592	7.0223	7.9654
0.44	1.1658	1.4769	1.8521	3.3250	4.9643	5.7147	6.8305	7.7846
0.45	1.1414	1.4582	1.8243	3.2354	4.8447	5.5950	6.7345	7.6989
0.46	1.1173	1.4394	1.7982	3.1497	4.7279	5.4771	6.6385	7.6160
0.48	1.0699	1.4018	1.7508	2.9896	4.5031	5.2470	6.4465	7.4569
0.50	1.0238	1.3641	1.7085	2.8436	4.2900	5.0250	6.2549	7.3050
0.55	0.9146	1.2708	1.6201	2.5337	3.8078	4.5077	5.7808	6.9456
0.60	0.8147	1.1795	1.5477	2.2898	3.3950	4.0462	5.3208	6.6004
0.65	0.7243	1.0913	1.4842	2.0980	3.0455	3.6403	4.8828	6.2596
0.70	0.6432	1.0071	1.4254	1.9468	2.7523	3.2875	4.4729	5.9200
0.80	0.5066	0.8526	1.3135	1.7306	2.3048	2.7235	3.7510	5.2485
0.90	0.3997	0.7179	1.2041	1.5867	1.9971	2.3149	3.1645	4.6081
1.00	0.3166	0.6027	1.0968	1.4822	1.7846	2.0226	2.7032	4.0232
1.10	0.2523	0.5056	0.9932	1.3979	1.6346	1.8134	2.3482	3.5087
1.20	0.2023	0.4245	0.8951	1.3235	1.5242	1.6616	2.0784	3.0699
1.30	0.1634	0.3570	0.8036	1.2535	1.4383	1.5482	1.8744	2.7041
1.40	0.1329	0.3009	0.7196	1.1855	1.3670	1.4601	1.7194	2.4046
1.50	0.1088	0.2545	0.6431	1.1187	1.3041	1.3882	1.6003	2.1621
1.60	0.0898	0.2160	0.5741	1.0530	1.2461	1.3262	1.5068	1.9674
1.70	0.0745	0.1840	0.5123	0.9887	1.1907	1.2704	1.4313	1.8114
1.80	0.0623	0.1573	0.4571	0.9262	1.1368	1.2182	1.3682	1.6862
1.90	0.0523	0.1350	0.4080	0.8658	1.0840	1.1682	1.3135	1.5851
2.00	0.0443	0.1163	0.3644	0.8080	1.0322	1.1195	1.2643	1.5025
2.50	0.0207	0.0584	0.2107	0.5624	0.7906	0.8898	1.0539	1.2405
3.00	0.0108	0.0318	0.1265	0.3880	0.5909	0.6888	0.8651	1.0683
3.50	0.0061	0.0186	0.0791	0.2693	0.4376	0.5257	0.6967	0.9148
4.00	0.0037	0.0115	0.0514	0.1895	0.3245	0.3995	0.5546	0.7726
5.00	0.0016	0.0050	0.0240	0.0988	0.1826	0.2334	0.3482	0.5357
6.00	0.0008	0.0025	0.0125	0.0552	0.1073	0.1408	0.2212	0.3667

Table 5. *Electron scattering factors $f_{el}(s)$ at $s = 0$*

Element	DHF[(a)]	DHF[(b)]	DHF[(c)]	HF[(a)]
He	0.41795	0.4173	0.418	0.41799
Li^+	0.51707	0.1569	0.517	0.51710
Li	3.28601	3.2556	3.286	3.28655
Be^{2+}	0.08175	0.0817	0.082	0.08179
Be	3.05381	3.0383	3.052	3.28655
B	2.79486	2.7850	2.794	2.79600
C(val.)	2.38750			2.38827
C(1*c*)	2.50569	2.4709	2.509	
C	2.43168			2.43283
N(1*c*)	2.21299	2.2034	2.211	
N	2.13023			2.13123
O(1*c*)	1.98058	1.9839	1.983	
O	1.96474			1.97006
F	1.80392	1.8017	1.801	1.80520
F^-	2.81839	2.6159		2.81873
Ne	1.65183	1.6494	1.652	1.65312
Na^+	1.12980	1.1285	1.130	1.13123
Na	4.77955	4.7387	4.778	4.79003
Mg^{2+}	0.83084	0.8300	0.831	0.83231
Mg	5.20917	5.1781	5.209	5.22318
Al	5.88978	5.8665	5.889	5.90498
Si(val.)	5.70553			5.71414
Si(1*c*)	5.81892	5.7535	5.828	
Si	5.67524			5.69046
P(1*c*)	5.49238	5.4738	5.488	
P	5.32942			5.34022
S(1*c*)	5.15450	5.1640	5.161	
S	5.13508			5.14397
Cl	4.86151	4.8566	4.857	4.87417
Cl^-	6.76674	6.3858	6.770	
Ar	4.58132	4.5712	4.580	4.59221

(*a*) Present calculation. (*b*) Rez *et al.* (1994). (*c*) Doyle & Turner (1968).

entos, Bunge & Cogordan, 1992; Bunge, Barrientos & Bunge, 1993), clarifying the opposite results of an early relativistic calculation (Mohanty & Clementi, 1989).

The reliability of the present method may be tested by considering the DHF solution for the ground state of N. From (10), the DHF wave function may be written as

$$\Psi = 1s^2 2s^2 2p^2 2P c_1 + 1s^2 2s^2 2p 2P^2 c_2 + 1s^2 2s^2 2P^3 c_3. \qquad (12)$$

The converged coefficients c_1, c_2 and c_3 have been found to be 0.472922, 0.745349 and 0.469892, respectively, in good agreement with the numerical solutions of Desclaux (1975), 0.472959, 0.745349 and 0.469857 and also with those given in (10). The total energy obtained, -54.43247077 hartree (1 hartree = 2643.6 kJ mol^{-1}), deviates from the previous value, -54.43247176 hartree, by only about one μhartree (better agreement is precluded by the lack of knowledge of the value of *c* used in the earlier calculation).

The DHF calculation for cations is straightforward after identifying the electron configuration of the ions. For the anions, we include only those that are stable at the DHF level of treatment since the choice of Watson-sphere radii (Watson, 1958) is quite arbitrary. The valence states of C and Si (quintet *S* states) have also been studied and the results are presented in the tables [labeled (val.)].

3.2. *Relativistic X-ray scattering factors of He–Ar*

The multiconfiguration DHF X-ray scattering factors are given in Tables 2–4. The agreement with previous tabulations (Doyle & Turner, 1968; Rez, Rez & Grant, 1994) for those single-configuration states is quite satisfactory. In fact, the deviations of the present values from those given by Doyle & Turner (1968; see also Maslen, Fox & O'Keefe, 1992) occur in the last significant figure for the first-row elements and the deviations increase a little when we move to the second-row elements. It also has been found that, in general, the present tabulations are closer to those given by Doyle & Turner (1968) than to the recent ones by Rez *et al.* (1994). For C, N, O, Si, P and S, we reproduced the early tabulations to comparable accuracy by employing single-configuration wave functions.

No separate tabulation of electron scattering factors is given as they can be obtained *via* the Mott formula [(3)]. We only give the electron scattering factor at $s = 0$ in Table 5. $f_{el}(0)$ is an important quantity as it can be used to predict the mean inner potential for a finite crystal and the latter quantity can be measured through electron holography (Gajdardziska-Josifovska *et al.*, 1993). We have used (4) to compute $f_{el}(0)$ for both neutral and charged elements. Nonrelativistic HF $f_{el}(0)$ has also been calculated and the results are summarized in Table 5. The overall agreement of the present DHF $f_{el}(0)$ with those tabulated before is reasonably good but in general it is closer to those given by Doyle & Turner (1968) than to the ones by Rez *et al.* (1994). Compared with the nonrelativistic HF value, $f_{el}(0)$ decreases as the relativistic effects have been taken into account.

Meyer *et al.* (1995) obtained a new set of X-ray scattering factors for He–Ar by treating the relativistic and correlation effects in an additive manner. They found the relativistic effects by taking the difference of X-ray scattering factors based on DHF wave functions (Doyle & Turner, 1968; Maslen, Fox & O'Keefe, 1992) and those based on HF wave functions (Tavard, Nicolas & Rouault, 1967; Wang, Sagar, Schmider & Smith, 1993). As discussed above, the earlier DHF X-ray scattering factors were obtained with single- or average-energy multiconfiguration wave functions, whereas for C, N, O, Si, P and S there is no direct relation between those DHF and HF wave functions as they are not referring to the same state. Thus, the previous results do not reflect genuine relativistic effects. In fact, in Fig. 3 of Meyer *et al.* (1995), the above six elements display completely different features from all the other elements. We have used the scattering factors from multiconfiguration wave functions to extract the differences and they are plotted in Fig. 1. It is clear that, in contrast with earlier studies, C, N, O, Si, P and S have features similar to those of the other elements within the same period.

We have also plotted the difference of X-ray scattering factors from a single-configuration DHF wave function and the HF ground states (Fig. 2 for C, N and O and Fig. 3 for Si, P and S). They resemble those reported by Meyer *et al.* (1995). A negative peak is found at around 0.2 Å^{-1} for C, N and O and at around 0.1 Å^{-1} for Si, P and S. The latter also show positive peaks at around 0.3 and 1.0 Å^{-1}.

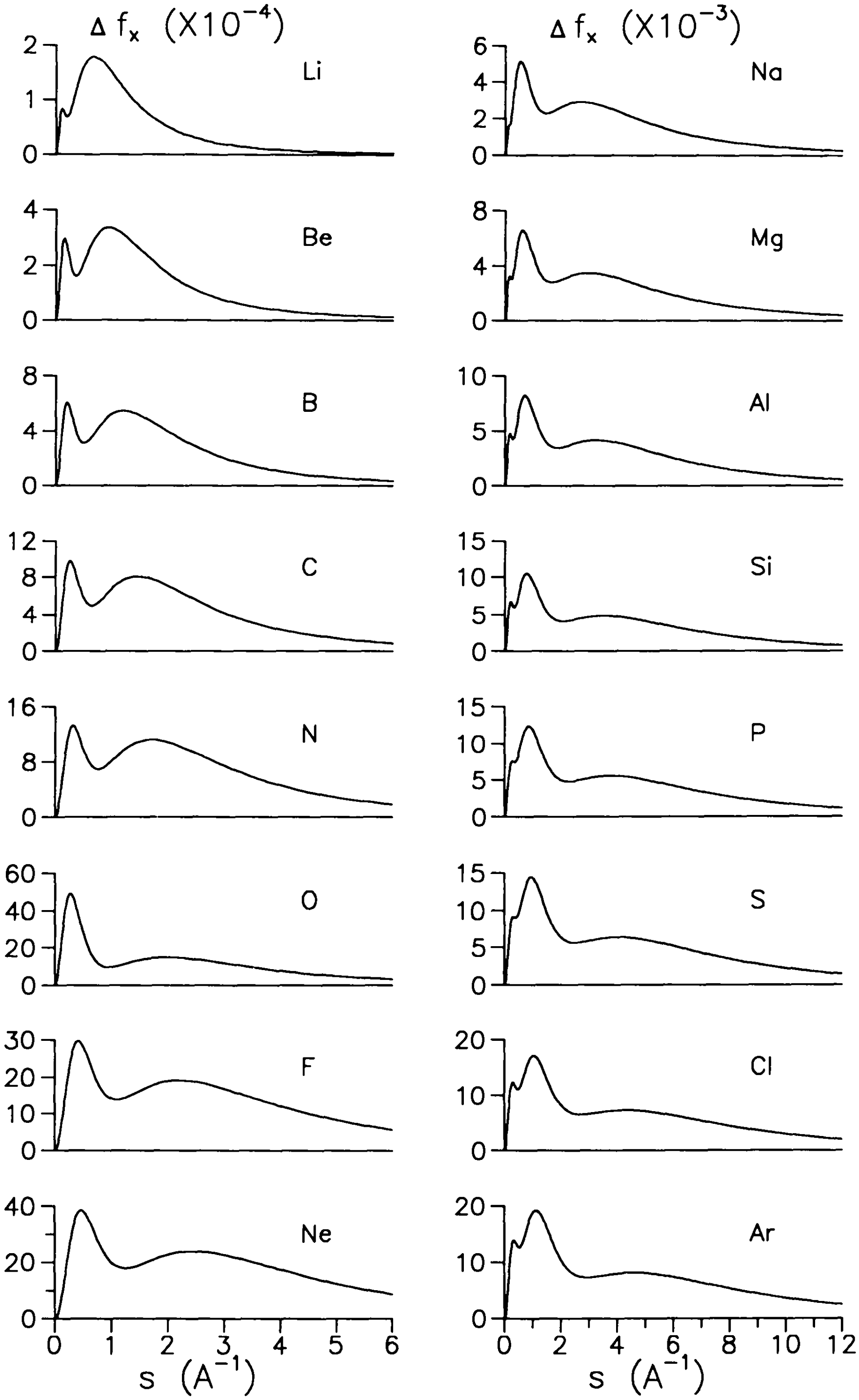

Fig. 1. Relativistic shifts [$\Delta f_x(s) = f_x^{\mathrm{DHF}}(s) - f_x^{\mathrm{HF}}(s)$] on X-ray scattering factors of He–Ar. Single-configuation DHF wave functions are used for all elements except C, N, O, Si, P and S, for which MCDHF wave functions are used.

There is another problem associated with the earlier study (Meyer, Müller & Schweig, 1995). Since the earlier tabulation of DHF X-ray scattering factors (Doyle & Turner, 1968; Maslen, Fox & O'Keefe, 1992) is given on a crude grid, the interpolation done by Meyer *et al.* (1995) failed to catch all the fine structures portrayed in Fig. 1. For instance, the inner peak is missing in the previous study [*cf.* Fig. 1 with Fig. 3 of Meyer *et al.* (1995)]. The present plot clearly shows the shell structure of the elements studied. A double-peak feature for the first-row elements and a triple-peak feature for the second-row elements are very prominent. In addition, the locations of the peaks move towards higher s as the nuclear charge increases. For the first-row elements, the inner peak moves from 0.1 in Li to 0.45 Å^{-1} in Ne, whereas the outside peak gradually shifts from 0.65 to 2.45 Å^{-1}. The three peaks in the second-row elements appear in the ranges 0.1–0.35, 0.55–1.15 and 2.75–4.5 Å^{-1}, respectively.

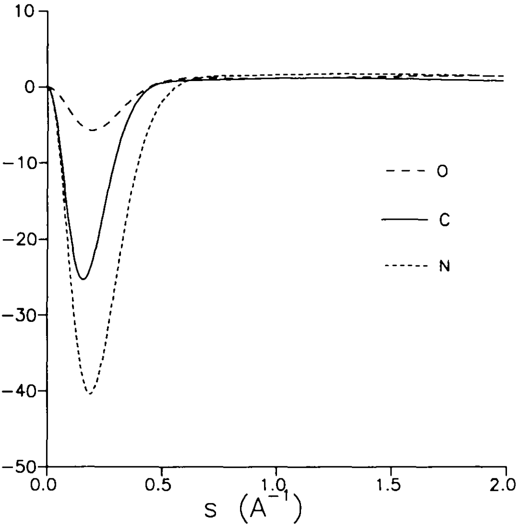

Fig. 2. Differences of X-ray scattering factors based on single-configuration DHF and HF wave functions [$\Delta f_x(s) = f_x^{\rm DHF}(s) - f_x^{\rm HF}(s)$] for C, N and O ground states.

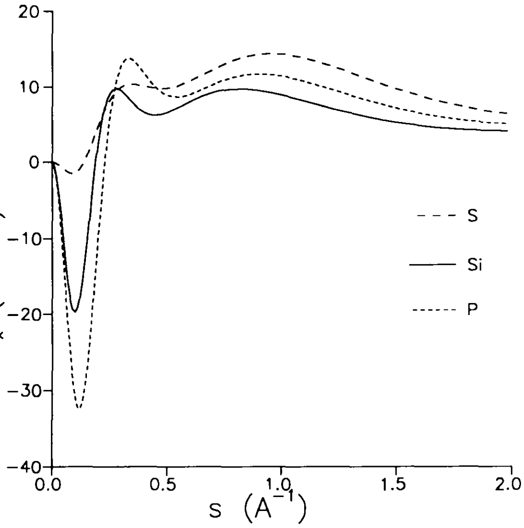

Fig. 3. Differences of X-ray scattering factors based on single-configuration DHF and HF wave functions [$\Delta f_x(s) = f_x^{\rm DHF}(s) - f_x^{\rm HF}(s)$] for Si, P and S ground states.

To illustrate the changes of electronic structures due to the inclusion of relativistic effects, we have plotted the radial density [$D(r) = 4\pi r^2\rho(r)$] differences between the relativistic and nonrelativistic P and Ar states in Fig. 4. They are consistent with the notion that the core electrons contract due to relativistic effects. Redistribution of electrons among different shells is responsible for the other details shown in Fig. 4. We have not seen any extra valence-electron-density expansion in P as speculated by Meyer *et al.* (1995).

The present tabulation of relativistic scattering factors should provide a good description of Rayleigh scattering for small momentum transfers and photon energies well above the K threshold of the target system. When the photon energy is close to the K threshold, the energy-dependent anomalous-scattering terms become important and modifications have to be made to account for the experiment. For more details on the applicability of elastic scattering factors and different modification schemes, we suggest that readers consult the comprehensive review by Pratt (1990).

4. Conclusions

X-ray and electron scattering factors have been calculated with a multiconfiguration DHF method by employing wave functions that yield the corresponding

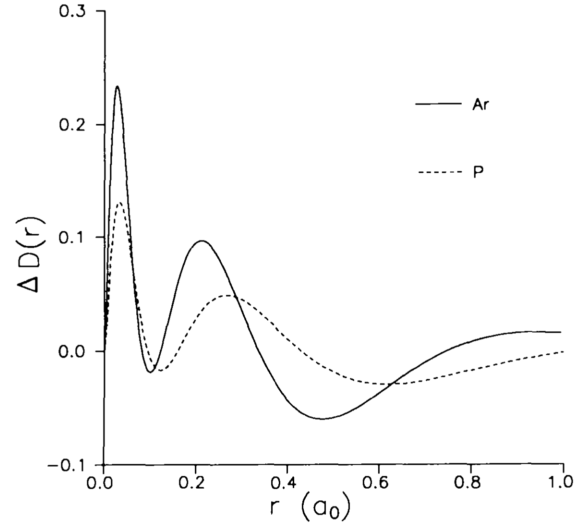

Fig. 4. Relativistic shifts [$\Delta D(r) = D^{\rm DHF}(r) - D^{\rm HF}(r)$] on the radial electron charge densities of P and Ar. The single-configuration DHF wave function is used for Ar and the MCDHF wave function is used for P.

nonrelativistic HF ground states as the speed of light goes to infinity. Thus, the difference between the present DHF scattering factors and the HF ones reflects genuine relativistic effects in contrast with earlier single- or average-energy multiconfiguration DHF calculations. The previously observed anomalous behavior for C, N, O, Si, P and S has been found to be due to an inconsistent treatment of these systems at the HF and DHF levels. With properly constructed multiconfiguration DHF wave functions, the energies of all of the first- and second-row elements and ions are lower than the corresponding nonrelativistic HF ground states, as expected, and distinct from the earlier work. The relativistic effects on X-ray scattering factors follow a gradual change as the nuclear charge increases.

The present tabulation will allow a better construction of high-quality X-ray scattering factors when taking the relativistic and correlation effects into account in an additive manner. Also, the use of a fine grid will avoid possible loss of important features due to interpolation.

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References

Bunge, C. F., Barrientos, J. A. & Bunge, A. V. (1993). *At. Data Nucl. Data Tables*, **53**, 113–162.

Bunge, C. F., Barrientos, J. A., Bunge, A. V. & Cogordan, J. A. (1992). *Phys. Rev. A*, **46**, 3691–3696.

Bunge, C. F., Jáuregui, R. & Ley-Koo, E. (1996). Preprint FT96–1, Instituto de Física, UNAM, Mexico.

Cohen, E. R. & Taylor, B. N. (1987). *Rev. Mod. Phys.* **59**, 1121–1148.

Coulthard, M. A. (1967). *Proc. Phys. Soc.* **91**, 44–49.

Desclaux, J. P. (1975). *Comput. Phys. Commun.* **9**, 31–45.

Doyle, P. A. & Turner, P. S. (1968). *Acta Cryst.* **A24**, 390–397.

Gajdardziska-Josifovska, M., McCartney, M. R., de Ruijter, W. J., Smith, D. J., Weiss, J. K. & Zuo, J. M. (1993). *Ultramicroscopy*, **50**, 285–299.

Grant, I. P., McKenzie, B. J., Norrington, P. H., Mayers, D. F. & Pyper, N. C. (1980). *Comput. Phys. Commun.* **21**, 207–231.

Ibers, J. A. (1958). *Acta Cryst.* **11**, 178–183.

Ishikawa, Y., Binning, B. C. Jr & Sando, K. M. (1983). *Chem. Phys. Lett.* **101**, 111–114.

Jáuregui, R., Bunge, C. F. & Ley-Koo, E. (1995). *AIP Conf. Proc.* No. 342, pp. 147–153. New York: American Institute of Physics.

Lee, Y. S. & McLean, A. D. (1982). *J. Chem. Phys.* **76**, 735–736.

Maslen, E. N., Fox, A. G. & O'Keefe, M. A. (1992). *International Tables for Crystallography*, Vol. C, edited by A. J. C. Wilson, Section 6.1.1, pp. 476–511. Dordrecht: Kluwer.

Meyer, H., Müller, T. & Schweig, A. (1995). *Acta Cryst.* **A51**, 171–177.

Mizushima, M. (1970). *Quantum Mechanics of Atomic Spectra and Atomic Structure*. New York: W. A. Benjamin.

Mohanty, A. K. & Clementi, E. (1989). *Chem. Phys. Lett.* **157**, 348–352.

NAG (1984). The IBM Double Precision Implementation of the NAG Fortran Library. Numerical Algorithms Group, Mark 11, Oxford, England.

Pratt, R. H. (1990). *X-ray and Inner-Shell Processes*, edited by T. A. Carlson, M. O. Krause & S. T. Manson. *AIP Conf. Proc.* No. 215, pp. 87–93. New York: American Institute of Physics.

Rez, D., Rez, P. & Grant, I. (1994). *Acta Cryst.* **A50**, 481–497.

Stanton, R. E. & Havriliak, S. (1984). *J. Chem. Phys.* **81**, 1910–1918.

Su, Z. & Coppens, P. (1994). Sagamore XI: Charge, Spin and Momentum Densities, Brest, France. Abstract Book.

Tavard, C., Nicolas, D. & Rouault, M. (1967). *J. Chim. Phys.* **64**, 540–554.

Thakkar, A. J. & Smith, V. H. Jr (1992). *Acta Cryst.* **A48**, 70–71.

Wang, J., Esquivel, R. O., Smith, V. H. Jr & Bunge, C. F. (1995). *Phys. Rev. A*, **51**, 3812–3818.

Wang, J., Sagar, R. P., Schmider, H. & Smith, V. H. Jr (1993). *At. Data Nucl. Data Tables*, **53**, 233–269.

Watson, R. E. (1958). *Phys. Rev.* **111**, 1108–1110.