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Abstract

Results of a preliminary study of the use of a model potential approach to the calculation of energy levels and radiative transition probabilities for highly ionized heavy atoms are reported. The calculations were carried out for eight ions in the sodium isoelectronic sequence from Mg II through W LXIV. The technique used involved the solution of the Dirac equation for the single outer valence electron, with a model central potential containing two disposable parameters affecting the potential in the region of the atomic core. The effect of core polarization was incorporated in the model potential. The parameters in the model potential were chosen by an initial solution of the non-relativistic Schrödinger equation for the single outer valence electron, with the requirement that calculated ionization energies reproduce the results of the best available non-relativistic calculations. Comparison of results for non-relativistic radiative transition probabilities provides the first check on the technique. Solutions of the Dirac equation are then compared with the results of other relativistic calculations and experimental measurements. The results, for both energy levels and radiative transition probabilities, are encouraging, and suggest that the wave functions obtained will be quite satisfactory for subsequent calculations of electron impact excitation of these ions.

I. Introduction

The goal of this project is progress toward a capability for carrying out calculations of electron impact excitation of highly ionized heavy atoms. The basic approach being investigated is based on model potential theory, which combines undisputed simplicity with accuracy potentially greater than that of an ab initio approach. This can be achieved through the incorporation of empirical data in the development of the model potentials, which may more than compensate for the formal approximations inherent in basic theoretical approach.

The first stage in this approach is the production of a reliable set of wave functions for the electronic states involved in the collision process. Experimental data on energy levels usually provides the basic data to be used in the development of such wave functions, and the associated model potentials. Unfortunately, experimental data of sufficient scope and precision is available only for atoms in relatively low stages of ionization. Thus, while relativistic effects are clearly important for highly ionized atoms, and must be accounted for in both the atomic structure and, ultimately, the collision calculations, the model potentials must be developed in a regime where relativistic effects are relatively unimportant.

We are constrained, therefore, to develop the model potentials in such a way that they can be extrapolated from the essentially non-relativistic regime to the regime where relativistic effects are important. This suggests study of an entire isoelectronic sequence, e.g. Na- or Mg-like ions, with a formulation of the model potential in which the parametric dependence is both relatively simple and confined to the non-relativistic aspect of the potential.

In order to be useful, the model potentials and wave functions must, at a minimum, be capable of yielding energy levels for states other than those

used in their development. The calculation of radiative transition probabilities provides for an even more stringent test. Again it is only in the essentially non-relativistic regime that data on radiative transition probabilities is abundant and very precise.

In the light of the above, we therefore decided to carry out a preliminary study based on determining the disposable parameters in the model potential with reference to the most accurate results available of ab initio non-relativistic calculations for energy levels. The wave functions so obtained could then be used to calculate radiative transition probabilities for comparison with the results of the same ab initio calculations, thereby providing an unambiguous check on the technique. This stage of the work is discussed in Section II.

The next stage involved using the model potential so obtained as the central potential in the Dirac equation for the outer valence electron. Energy levels and radiative transition probabilities so obtained are compared with those of other ab initio calculations and experimental measurements in Section III. Conclusions and the implications for future work are discussed in Section IV.

II. Non-relativistic Calculations

The model non-relativistic Schrodinger equation for the outer valence electron of a sodium-like ion involves the equation

$$\left[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} + V(r) + \epsilon_{n\ell} \right] P_{n\ell}(r) = 0 \quad (1)$$

for the radial part of the wave function for the state with quantum numbers n and ℓ and energy $\epsilon_{n\ell}$. We use atomic units throughout, i.e., r is in units of a_0 and $\epsilon_{n\ell}$ in Rydberg. The potential $V(r)$ incorporates the interactions with all of the other electrons and the nucleus, with limiting forms

$$\begin{aligned} V(r) &\underset{r \rightarrow 0}{\sim} \frac{2Z}{r} \\ V(r) &\underset{r \rightarrow \infty}{\sim} \frac{2z}{r}, \end{aligned} \quad (2)$$

where Z is the nuclear charge, and $z=Z-10$.

$$V(r) = V(\lambda, r) + V(r_c, r), \quad (3)$$

where $V(\lambda, r)$ is the scaled Thomas-Fermi-Dirac statistical model potential,¹ with limiting forms (2), and $V(r_c, r)$ is of the form

$$V(r_c, r) = \frac{\alpha_d}{r^4} W_6(r_c, r) + \frac{\alpha'_q}{r^6} W_{10}(r_c, r), \quad (4)$$

where

$$W_m(r_c, r) = \left[1 - e^{-(r/r_c)^m} \right], \quad (5)$$

and α_d and α'_q are the dipole and effective quadrupole polarizabilities of the ionic core, respectively. [We use the word "effective" with respect to the quadrupole term, as it may also include a contribution from dynamic effects in the dipole interaction which go as r^{-6} at long distances.]

The two disposable parameters in the present calculations are the scale factor λ in $V(\lambda, r)$, which is of order unity, and the short-range cut-off radius r_c in $V(r_c, r)$, which is of order the radius of the core. We may choose λ and r_c to be functions of ℓ , but not n , without in any way complicating the calculations. It should be noted at the outset that the present choice for $V(r)$ is somewhat arbitrary, in that other forms of the model potential might be contemplated.

The results of the very elaborate ab initio non-relativistic configuration interaction (CI) calculations of Froese Fischer² for the ionization energies of ions from Mg II through Fe XVI were used to determine the parameters λ and r_c in $V(r)$ for ions with $Z \leq 26$. Since results were available for two states in each of the series ns^2S and np^2P , we obtained λ and r_c separately for each series. For ions with $Z > 26$ we used the results of the non-relativistic Hartree-Fock calculations of Weiss³ for the states $3s^2S$ and $3p^2P$, after adding estimates of the correlation energy corrections (less than 0.03 a.u.) obtained by extrapolation of the values given by Froese Fischer for ions with $Z \leq 26$, which were fitted to the expansion $E_0 + E_1/Z + E_2/Z^2$. Since only one state in each series is known accurately, the values of r_c were extrapolated from the results for $Z \leq 26$, which were found to behave as $(Z-5)^{-1}$. The values of λ for the s and p series were then obtained with reference to the $3s^2S$ and $3p^2P$ states.

The polarizabilities α_d and α_q used in $V(r_c, r)$ were taken from analyses of spectral data for Mg II⁴ and Si IV.⁵ These data, along with similar results for P V⁶ and Ti XII⁷ were used to obtain values for all other ions considered by extrapolation according to the formulae⁴

$$\alpha_d = A(Z)/z^4 = c/(Z-s)^4 \quad (6)$$

and

$$\alpha'_q = k(Z)A(Z)/z^6 \quad (7)$$

where

$$k(Z)/\sqrt{A(Z)} = a+bz, \quad (8)$$

a, b, c and s are disposable constant parameters.

The energy levels used in this fitting process and the parameters obtained are given in Table I. This set of parameters was used in all subsequent calculations reported here. [More accurate results for α_d and α'_q for ions with $Z \geq 19$ have recently been presented⁸ based on new analyses of the spectra of K IX and Ca X, which should be used in any future work.]

The results of these completely non-relativistic calculations were used to calculate radiative transition probabilities for the lowest three s and p states of these ions. The effect of core polarization is included in the dipole matrix element,⁹ which may be written

$$\vec{M}_{if} = \langle \psi_f | \vec{r} \left[1 - \frac{\alpha_d}{r^3} \bar{W}_3(r_c^i, r_c^f, r) \right] | \psi_i \rangle \quad (9)$$

where

$$\bar{W}_3(r_c^i, r_c^f, r) = \frac{1}{2} \left[W_3(r_c^i, r) + W_3(r_c^f, r) \right]. \quad (10)$$

The form of the cut-off function $\bar{W}$ in (9) is chosen to be consistent with that used in $V(r_c, r)$.

The results are given in Table II and III, from calculations both with and without the core polarization term in (9). The results f_1 of Froese Fischer² were not obtained with the simple approximation (9), but from a thorough study of the effect of including excited core configurations in the CI wave functions. The agreement between the present results and those of these much more elaborate calculations is seen to be generally excellent, for both f_0 and f_1 , except for

the very sensitive case of the 3s-4p transition in Mg II. Since the energies were chosen to be identical to those of Froese Fischer, dipole matrix elements are in equally good agreement.

These results confirm the conclusion of Froese Fischer that core polarization effects cannot account for the large discrepancy between calculated and measured lifetimes for the 3p state in the sodium isoelectronic sequence. [In the following section we will see that the hypothesis of Froese Fischer to the effect that relativistic effects cannot provide the explanation either is born out.] It has recently been shown¹⁰ that cascade effects unaccounted for in the analysis of the beam-foil data may provide the explanation.

For all the transitions considered, we see that core polarization effects for $Z > 26$ are generally small ($\lesssim 5\%$). But we do notice the curious effect that core polarization seems to introduce the largest correction for transitions involving the 5s state around $Z=26$. This is contrary to the trend for all other transitions, in which core polarization becomes a decreasingly important effect as the degree of ionization increases. This should perhaps serve as a warning in future work that core polarization may not necessarily be ignored for high stages of ionization simply because it is found to be a negligible effect for the first few ions in an isoelectronic sequence.

III. Relativistic Calculations

With the model potentials obtained from the non-relativistic calculations, we proceeded to solve the one-particle Dirac equation for the outer valence electron. The radial equations were taken to be¹¹

$$\left[\frac{d}{dr} + \frac{k}{r} \right] G = \frac{1}{\alpha} \left[\epsilon + \frac{\alpha^2}{2} V(r) + 1 \right] F, \quad (11)$$

and

$$\left[\frac{d}{dr} - \frac{k}{r} \right] F = - \frac{1}{\alpha} \left[\epsilon + \frac{\alpha^2}{2} V(r) - 1 \right] G, \quad (12)$$

where α is the fine structure constant, $V(r)$ is given by (3) and (13)

$$\epsilon = 1 + \frac{1}{2} \alpha^2 \epsilon_k, \quad (14)$$

where ϵ_k is in units of Rydberg, as before. The quantum number k takes on the values -1, 1 and -2 for the states of interest, i.e. $^2S_{1/2}$, $^2P_{1/2}$ and $^2P_{3/2}$, respectively.

The calculated ionization energies and fine structure splittings for the first three s and p states are compared with available spectroscopic data in Table IV. It is quite clear that for the lower stages of ionization, where the relativistic shifts and spin-orbit splittings are small, we have seriously over-estimated the former and underestimated the latter. For Ca X and Fe XVI, however, the discrepancies are much less. We have no explanation for this trend at present, but there would appear to be reasonable grounds for confidence in the results obtained for $Z > 26$.

Some of these results are given in Table V, where they are compared with the results of the calculations by Weiss.³ These latter are based on non-relativistic single-configuration Hartree-Fock wave functions, which are used to calculate the dominant relativistic corrections from the Pauli Hamiltonian by perturbation theory. The best agreement between the two calculations seems to occur at Kr XXVI, but agreement worsens noticeably thereafter.

Let us consider in a little more detail the fine structure splittings of the 3p doublet, which have been calculated by a variety of techniques, and for which some experimental data is available. These are given in Table VI. The two calculations other than the present and HFP should be more accurate. Those of Cowan¹⁵ somewhat improve on the HFP approach, in that some relativistic corrections from the Pauli Hamiltonian are added to the non-relativistic Hamiltonian, which is used to obtain radial wave functions. In this approach only the spin-orbit interaction is treated by perturbation theory. The Dirac-Hartree-Fock results of Kim¹⁶ should be the most accurate of all.

We see that with the curious exception of Fe XVI, the HFR results seem to be in better agreement with the DHF results than are the HFP results, as expected. The DHF results also seem to be in the best agreement with experimental measurements given that the data Mo XXXII has the largest experimental uncertainty. Thus it is with some satisfaction that we note the increasingly good agreement between the present results and the DHF results for larger Z .

The wavelengths of the resonance transitions $3s_{1/2}-3p_{1/2,3/2}$ are also interesting, and are compared with the results of the other calculations and experimental measurements in Table VII. We see that the agreement between the measured values for $3s_{1/2}-3p_{1/2}$ and all of the calculations except the DHF is reasonably good. Furthermore, all of the calculations except the DHF seem to be in good agreement for high Z . For the $3s_{1/2}-3p_{3/2}$ transition the same holds for low Z , but for high Z the HFP results diverge from those of the other calculations.

There are also some results available for W LXIV from another Dirac-Hartree-Fock calculation,¹⁷ which may differ from the program of Kim in very subtle magnetic and retardation corrections. These results, both for the fine-structure splitting (27.41 Ryd) and the wavelengths of the 3s-3p transitions (75.27Å and 23.06Å) are in excellent agreement with those of Kim.

The only other relativistic results known to us are the Mo XXXII from a variational model potential approach.¹⁸ The fine-structure splitting (2.00 Ryd) and wavelengths of the 3s-3p transitions (175.94Å and 126.97Å) are in best agreement with the DHF results.

Turning now to the calculated radiative transition probabilities for $Z \geq 26$, we compare the results of the present calculations with those of others in Table VIII. In order to eliminate the effect of calculated wavelengths, we present line strengths, scaled by Z^2 for convenience, rather than oscillator strengths. The relation between the two is

$$f = \frac{\Delta \epsilon}{3\omega} S, \quad (15)$$

where ω is the statistical weight of the initial state.

First we note that the agreement between the non-relativistic model potential (NRMP₀) and Hartree-Fock (NRHF₀) results, where both neglect the effect of core polarization, is excellent. This confirms the conclusions reached in Section II that the model potential approach can faithfully reproduce the ab initio results, when the energy levels of the latter are used as the data on which the former is based.

Considering the relativistic Hartree-Fock results of Cowan, we note the progressive deviation from the non-relativistic results as Z increases, but that the ratio of the line strengths for 3p_{1/2} and 3p_{3/2} is constant at 2.0.

This reflects the fact that the HFR approach uses the same radial wave function for both members of the p-doublet, but does include relativistic effects other than the spin-orbit interaction in obtaining these wave functions.

The DCHF₀ and DHF₀ results include the effect of the spin-orbit interaction on the radial orbitals. In the DCHF approach this is carried out by using the HFP wave functions to calculate the dipole matrix element, which is then corrected using information obtained from exact solutions of the Dirac equation for hydrogenic ions.¹⁹ The DHF calculations include this effect directly, of course, and the two approaches are seen to yield nearly identical results.

Comparison of either, then, with the HFR results yields a measure of the effect of the spin-orbit interaction alone on the line strengths. It would appear that the 3s_{1/2}-3p_{1/2} transition is much more affected than the 3s_{1/2}-3p_{3/2} transition. The reason for this behavior is not immediately obvious.

Finally, considering the results of the Dirac model potential calculations (DMP₀), we note that they are generally in excellent agreement with the DCHF and DHF results, and seem to faithfully reflect the changes due to relativistic effects.

The final column contains results obtained including the effect of core polarization in the dipole matrix elements. For $Z \leq 36$ this effect is seen to be of importance comparable or greater than the relativistic effect, but becomes negligible by comparison for high Z . This is generally true for all transitions studied.

The results given in Table IX speak to the question of the importance of relativistic effects on oscillator strengths for $Z \leq 26$. For all the transitions listed the effect is only on the order of a few percent. For the resonance transition, the effect is to further increase the oscillator

strengths, which are already some 20-30% larger than the results of beam foil measurements. Thus relativistic effects cannot explain this large discrepancy.

In Tables X and XI we collected all of the results from the present calculations, for transition wavelengths and oscillator strengths. The former are compared with experimental data, where available. The oscillator strengths were obtained from the line strengths using the calculated wavelengths.

IV. Summary and Conclusions

The aim of the model potential approach is to obtain simple wave functions for the valence electrons in heavy atoms or molecules. The manner in which the method is applied depends mainly on the availability of reliable theoretical or experimental data on the systems of interest. For the ions in the Na sequence this data presently includes:

- 1) Non-relativistic multi-configuration Hartree-Fock calculations by Froese Fischer² of energy levels and oscillator strengths in several ions from Mg II through Fe XVI,
- 2) Single configuration calculations by Weiss³, Cowan¹⁵ and Kim¹⁶ for selected ions with high Z. These calculations differ in their treatment of relativistic effects (see Table VI).
- 3) Measurements of transition probabilities for the lightest ions, and transition energies for ions up to Mo XXXII.

In the present calculations the model potential parameters were based on the non-relativistic calculations by Froese Fischer² and Weiss³. Two alternative choices were considered. The use of relativistic calculations could perhaps have led to a more accurate representation of the effects of the spin-orbit forces. However the ab initio relativistic calculations that are available at this time show some inconsistencies, and they all ignore the effects of core polarization. The use of experimental data on transition wavelengths would be difficult since there is only limited information on most members of the sequence, and none for the ions with very high Z. Extrapolation of potential parameters from low-Z to high-Z would be necessary and such extrapolation could be very dangerous since

the relativistic effects are relatively small in the ions for which data is available.

Our principal aim was thus to study the feasibility of using non-relativistic calculations as the basis for the construction of model potentials. Our conclusions in this regard are:

1) The model potential method permits one to determine, in a very simple manner, the effects of core polarization on valence orbitals. This conclusion is supported by the results shown in Tables II, III & IX. The significance of core polarization in ions with high Z can be assessed from Table VIII.

2) If one substitutes a potential that is deduced from non-relativistic calculations into the Dirac equation for a valence electron, the calculated fine structure splittings are too small. The relative error decreases with increasing Z , and is $\sim 3\%$ for Kr XXVI.

3) The comparison of the results of four relativistic calculations in Tables VII and VIII shows that there are uncertainties of up to 15% in the wavelengths and line-strengths of the two lowest resonance lines. Until the differences between the ab initio calculations are understood it is not possible to assess fully the accuracy of the model potential method.

It could be argued that the model potential calculations of transition probabilities are the best available, since they include both relativistic effects and core-polarization. However such an advantage is probably only transitory and the major value of this approach lies in the study of other properties of highly charged ions, such as the interactions with electrons and other ions. We hope that it will be possible to extend this work and recommend that the study of electron collisions be undertaken

soon. The level of accuracy that has been demonstrated in this work supports the thesis that in many collision processes the presence of the core electrons can be simulated by a model potential, with a considerable saving in computational time.

Table I. Data (see text for sources) used for constructing model potentials. Ionization energies are in units of the atomic Rydberg, polarizabilities are in a.u.

	I(3s)	I(4s)	I(3p)	I(4p)	α_d	α'_q	λ^0	λ^1	r_c^0	r_c^1
Mg II	1.10412	0.46872	0.77894	0.37014	4.696(-1)	6.20(-1)	0.76495	0.83436	0.6680	0.7260
Si IV	3.31274	1.54842	2.66268	1.32690	1.489(-1)	2.06(-1)	0.82779	0.86184	0.5338	0.5486
Ca X	15.46466	7.91454	13.88556	7.31098	1.70(-2)	1.50(-2)	0.88613	0.89936	0.3198	0.3165
Fe XVI	35.69212	18.83472	33.20750	17.84568	4.19(-3)	2.69(-3)	0.91179	0.91555	0.2295	0.2234
Kr XXVI	87.242		83.258		8.57(-4)	3.84(-4)	0.92179	0.93352	0.1548	0.1516
Mo XXXII	128.846		123.968		4.16(-4)	1.57(-4)	0.92734	0.93978	0.1297	0.1270
Xe XLIV	236.066		229.394		1.33(-4)	3.83(-5)	0.93413	0.94658	0.0980	0.0959
W LXIV	485.88		476.22		3.33(-5)	6.85(-6)	0.93960	0.95223	0.0696	0.0681

Table II. Oscillator strengths from the present non-relativistic calculation compared with those from the calculation of Froese Fischer (F-F). Results neglecting core polarization are f_0 , results including core polarization f_1 .

	3s-3p		3s-4p		3p-4s		4s-4p	
	present	F-F	present	F-F	present	F-F	present	F-F
Mg II								
f_0	9.52(-1)	9.50(-1)	3.19(-4)	3.40(-4)	1.48(-1)	1.47(-1)	1.40	1.40
f_1	9.04(-1)	9.12(-1)	1.20(-3)	9.70(-4)	1.50(-1)	1.49(-1)	1.39	1.39
Si IV								
f_0	8.05(-1)	8.03(-1)	3.19(-2)	3.24(-2)	1.16(-1)	1.16(-1)	1.18	1.18
f_1	7.58(-1)	7.62(-1)	3.92(-2)	3.83(-2)	1.20(-1)	1.19(-1)	1.16	1.17
Ca X								
f_0	5.16(-1)	5.14(-1)	1.52(-1)	1.52(-1)	7.67(-2)	7.68(-2)	7.48(-1)	7.47(-1)
f_1	4.91(-1)	4.90(-1)	1.63(-1)	1.63(-1)	8.05(-2)	8.01(-2)	7.40(-1)	7.40(-1)
Fe XVI								
f_0	3.74(-1)	3.73(-1)	2.28(-1)	2.29(-1)	6.22(-2)	6.23(-2)	5.42(-1)	5.42(-1)
f_1	3.61(-1)	3.59(-1)	2.38(-1)	2.39(-1)	6.51(-2)	6.51(-2)	5.38(-1)	5.37(-1)
Kr XXVI								
f_0	2.56(-1)		3.01(-1)		5.15(-2)		3.70(-1)	
f_1	2.49(-1)		3.09(-1)		5.35(-2)		3.67(-1)	
Mo XXXII								
f_0	2.15(-1)		3.28(-1)		4.81(-2)		3.10(-1)	
f_1	2.10(-1)		3.35(-1)		4.98(-2)		3.09(-1)	
Xe XLIV								
f_0	1.63(-1)		3.64(-1)		4.40(-2)		2.35(-1)	
f_1	1.60(-1)		3.69(-1)		4.52(-2)		2.34(-1)	
Mo LXIV								
f_0	1.16(-1)		3.97(-1)		4.04(-2)		1.67(-1)	
f_1	1.15(-1)		4.01(-1)		4.13(-2)		1.67(-1)	

Table III. Additional oscillator strengths from the present non-relativistic calculation neglecting core polarization (f_0) and including core polarization (f_1).

		3s-5p	4s-5p	5s-5p	3p-5s	4p-5s
Mg II	f_0	1.13(-3)	1.14(-3)	1.82	1.80(-2)	2.68(-1)
	f_1	2.04(-3)	8.97(-4)	1.82	1.87(-2)	2.69(-1)
Si IV	f_0	1.46(-2)	2.35(-2)	1.53	1.78(-2)	2.06(-1)
	f_1	1.80(-2)	2.52(-2)	1.53	1.90(-2)	2.08(-1)
Ca X	f_0	5.03(-2)	1.55(-1)	9.69(-1)	1.42(-2)	1.33(-1)
	f_1	5.48(-2)	1.59(-1)	9.66(-1)	1.54(-2)	1.34(-1)
Fe XVI	f_0	6.95(-2)	2.43(-1)	7.01(-1)	1.23(-2)	1.06(-1)
	f_1	7.32(-2)	2.47(-1)	7.00(-1)	1.33(-2)	1.08(-1)
Kr XXVI	f_0	8.60(-2)	3.28(-1)	4.77(-1)	1.07(-2)	8.69(-2)
	f_1	8.86(-2)	3.32(-1)	4.76(-1)	1.14(-2)	8.78(-2)
Mo XXXII	f_0	9.17(-2)	3.60(-1)	4.00(-1)	1.02(-2)	8.08(-2)
	f_1	9.39(-2)	3.63(-1)	4.00(-1)	1.08(-2)	8.16(-2)
Xe XLIV	f_0	9.89(-2)	4.02(-1)	3.03(-1)	9.49(-3)	7.34(-2)
	f_1	1.01(-1)	4.04(-1)	3.03(-1)	9.94(-3)	7.40(-2)
W LXIV	f_0	1.05(-1)	4.41(-1)	2.15(-1)	8.88(-3)	6.72(-2)
	f_1	1.06(-1)	4.43(-1)	2.15(-1)	9.20(-3)	6.76(-2)

Table IV. Ionization energies and fine-structure splittings from the present calculation compared with experimental measurements, in units of the atomic Rydberg.

	Mg II		Si IV		Ca X		Fe XVI	
	exp. ^a	calc.	exp. ^b	calc.	exp. ^c	calc.	exp. ^d	calc.
3s1/2	1.10510	1.10577	3.31793	3.31998	15.52870	15.53778	35.9603	35.9846
4s1/2	0.46897	0.46920	1.55022	1.55076	7.93967	7.94256	18.9420	18.9525
5s1/2	0.25951	0.25960	0.89921	0.89944	4.82382	4.82523	11.7022	11.6987
3p1/2	0.78005	0.77977	2.66829	2.66705	13.94113	13.94286	33.4346	33.4537
3p3/2	0.77921	0.77911	2.66409	2.66362	13.89489	13.90135	33.2434	33.2754
Δ	0.00084	0.00068	0.00420	0.00343	0.04624	0.04151	0.1912	0.1783
4p1/2	0.37042	0.37043	1.32889	1.32856	7.33362	7.33417	17.9349	17.9499
4p3/2	0.37014	0.37021	1.32742	1.32732	7.31620	7.31805	17.8615	17.8789
Δ	0.00028	0.00022	0.00147	0.00124	0.01742	0.01612	0.0734	0.0710
5p1/2	0.21700	0.21702	0.79819	0.79807	4.53092	4.53156	11.1994	11.2043
5p3/2	0.21687	0.21692	0.79750	0.79748	4.52260	4.52366	11.1630	11.1689
Δ	0.00013	0.00010	0.00069	0.00059	0.00832	0.00790	0.0364	0.0354

a) Ref. 12

b) Ref. 5

c) Ref. 8

d) Ref. 13

Table V. Ionization energies and fine-structure splittings from the present calculations compared with the Hartree-Fock-Pauli (HFP) calculations of Weiss, in units of the atomic Rydberg.

	Fe XVI		Kr XXVI		Mo XXXII		Xe XLIV		W LXIV	
	present	HFP	present	HFP	present	HFP	present	HFP	present	HFP
3s1/2	35.9846	35.924	88.685	88.518	131.821	131.548	245.662	244.506	526.02	519.14
4s1/2	18.9525		47.679		71.287		133.591		285.89	
5s1/2	11.6987		29.750		44.616		83.821		179.16	
3p1/2	33.4537	33.394	84.560	84.378	126.701	126.400	238.283	237.192	514.70	507.74
3p3/2	33.2754	33.206	83.643	83.461	124.780	124.527	232.014	231.413	487.12	485.01
Δ	0.1783	0.188	0.917	0.917	1.921	1.873	6.269	5.779	27.58	22.73
4p1/2	17.9499	17.935	46.002	45.958	69.192	69.116	130.531		281.29	
4p3/2	17.8789	17.862	45.630	45.590	68.408	68.362	127.959		269.91	
Δ	0.0710	0.073	0.372	0.368	0.784	0.754	2.572		11.38	
5p1/2	11.2043	11.193	28.914	28.880	43.569	43.514	82.284		176.87	
5p3/2	11.1689	11.157	28.728	28.696	43.175	43.136	80.987		171.13	
Δ	0.0354	0.036	0.186	0.184	0.394	0.378	1.297		5.74	

Table VI. Fine-structure splitting of the 3p doublet from the present calculations compared with experimental measurements, the Hartree-Fock-Pauli (HFP) calculations of Weiss, the relativistic Hartree-Fock (HFR) calculations of Cowan, and the Dirac-Hartree-Fock (DHF) calculations of Kim, in units of the atomic Rydberg.

	exp.	present	HFP	HFR	DHF
Fe XVI	0.1912 ^a	0.178	0.188	0.185	0.190
Kr XXVI	0.943 ^b	0.917	0.919	0.941	0.945
Mo XXXII	1.92 ^b	1.92	1.87	1.97	1.96
Xe XLIV		6.27	5.78	6.45	6.31
W LXIV		27.6	22.7	29.0	27.4

a) Ref. 13

b) Ref. 14

Table VII. Wavelengths for the resonance transitions from the present calculation compared with the Hartree-Fock-Pauli (HFP) calculations of Weiss, the relativistic Hartree-Fock (HFR) calculations of Cowan, and the Dirac-Hartree-Fock (DHF) calculations of Kim, in Å.

	3s _{1/2} -3p _{1/2}					3s _{1/2} -3p _{3/2}				
	exp.	present	HFP	HFR	DHF	exp.	present	HFP	HFR	DHF
Fe XVI	360.8	360.1	360.2	361	358.8	335.4	336.4	335.3	337	333.8
Kr XXVI	220.6	220.9	220.1	221	218.0	179.6	180.7	180.2	180	177.8
Mo XXXII	177	178.0	177.0	178	174.5	129	129.4	129.8	129	126.9
Xe XLIV		123.5	124.6	126	121.6		66.77	69.6	66.5	66.00
W LXIV		80.55	79.9	80.0	74.96		23.42	26.7	22.6	23.01

Table VIII. Scaled line strengths Z^2S from the present non-relativistic (NRMP) and Dirac (DMP) model potential calculations compared with the non-relativistic Hartree-Fock (NRHF) and Dirac-corrected Hartree-Fock (DCHF) calculations of Weiss, the relativistic Hartree-Fock (HFR) calculations of Cowan, and the Dirac-Hartree-Fock (DHF) Calculations of Kim. The subscript 0(1) indicate that core polarization has been neglected (included).

	NRHF ₀	NRMP ₀	HFR ₀	DCHF ₀	DHF ₀	DMP ₀	DMP ₁
Fe XVI							
3s1/2-3p1/2	204.2	203.6	202	199.5	199.6	200.0	192.6
3s1/2-3p3/2	408.4	407.3	404	404.3	404.2	402.8	387.9
Kr XXVI							
3s1/2-3p1/2	166.4	166.5	163	159.7	161.0	160.6	156.2
3s1/2-3p3/2	332.8	333.1	326	326.5	327.8	326.4	317.6
Mo XXXII							
3s1/2-3p1/2	155.2	155.5	151	146.8	148.0	147.7	144.3
3s1/2-3p3/2	310.5	310.9	303	302.4	303.6	302.4	295.5
Xe XLIV							
3s1/2-3p1/2	142.3	142.4	136	129.5	130.8	130.2	127.8
3s1/2-3p3/2	284.6	284.8	271	272.4	272.4	271.3	266.6
W LXIV							
3s1/2-3p1/2	131.6	131.6	119	108.6	110.6	109.8	108.2
3s1/2-3p3/2	263.2	263.2	239	239.0	239.8	238.6	235.3

Table IX. Oscillator strengths for the entire multiplets from the present non-relativistic (NRMP) and Dirac model potential (DMP) calculations compared with those from the calculations of Froese-Fischer. All results include core polarization.

	Mg II	Si IV	Ca X	Fe XVI
<hr/>				
3s-3p				
NRMP	9.04(-1)	7.58(-1)	4.91(-1)	3.61(-1)
DMP	9.05(-1)	7.61(-1)	5.01(-1)	3.79(-1)
F-F	9.12(-1)	7.62(-1)	4.90(-1)	3.59(-1)
3s-4p				
NRMP	1.20(-3)	3.92(-2)	1.63(-1)	2.38(-1)
DMP	1.12(-3)	3.84(-2)	1.58(-1)	2.28(-1)
F-F	9.70(-4)	3.83(-2)	1.63(-1)	2.39(-1)
3p-4s				
NRMP	1.50(-1)	1.20(-1)	8.05(-2)	6.51(-2)
DMP	1.51(-1)	1.20(-1)	8.19(-2)	6.75(-2)
F-F	1.49(-1)	1.19(-1)	8.01(-2)	6.51(-2)
4s-4p				
NRMP	1.39	1.16	7.40(-1)	5.38(-1)
DMP	1.39	1.17	7.55(-1)	5.65(-1)
F-F	1.39	1.17	7.40(-1)	5.37(-1)
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Table X. Transition wavelengths from the present calculation compared with experimental measurements, in Å.

	Mg II		Si IV		Ca X		Fe XVI		Kr XXVI		Mo XLIV	
	exp. ^a	calc.	exp. ^b	calc.	exp. ^c	calc.	exp. ^d	calc.	exp. ^e	calc.	exp. ^e	calc.
3s1/2-3p1/2	2804	2795	1403	1396	574.0	571.4	360.8	360.1	220.6	220.9	177	178.0
-3p3/2	2796	2790	1394	1388	557.8	556.9	335.4	336.4	179.6	180.7	129	129.4
-4p1/2	1240	1239	458.2	457.6	111.2	111.1	50.57	50.53		21.35		14.55
-4p3/2	1240	1239	457.8	457.3	111.0	110.9	50.36	50.33		21.17		14.37
-5p1/2	1026	1025	361.7	361.3	82.86	82.80	36.80	36.77		15.25		10.33
-5p3/2	1026	1025	361.6	361.6	82.80	82.74	36.75	36.72		15.20		10.28
4s1/2-4p1/2	9247	9226	4117	4101	1504	1498	904.9	908.9		543.4		434.9
-4p3/2	9221	9206	4090	4078	1461	1459	843.4	848.7		444.6		316.5
-5p1/2	3617	3614	1212	1211	267.3	267.2	117.7	117.6		48.56		328.8
-5p3/2	3615	3612	1211	1210	266.7	266.5	117.1	117.1		48.08		324.1
5s1/2-5p1/2	21440	21400	9021	8989	3111	3103	1813	1843		1091		870.9
-5p3/2	21380	21350	8960	8938	3025	3022	1690	1720		891.6		632.4
3p1/2-4s1/2	2929	2934	815.0	816.4	151.8	151.9	62.87	62.84		24.71		16.44
-5s1/2	1751	1752	515.1	515.5	99.95	99.95	41.93	41.89		16.63		11.10
3p3/2-4s1/2	2937	2940	818.9	818.9	153.0	152.9	63.71	63.62		25.34		17.04
-5s1/2	1753	1754	516.3	516.5	100.5	100.4	42.30	42.23		16.91		11.37
4p1/2-5s1/2	8216	8223	2121	2124	363.1	363.2	146.2	145.8		56.07		37.08
4p3/2-5s1/2	8237	8239	2138	2130	365.7	365.6	148.0	147.5		57.39		38.30

a) Ref. 12

b) Ref. 5

c) Ref. 8

d) Ref. 13

e) Ref. 14

Table XI. Oscillator strengths from the present Dirac model potential calculation, including the effect of core polarization.

	Mg II	Si IV	Ca X	Fe XVI	Kr XXVI	Mo XXXII	Xe XLIV	W LXIV
3s1/2-3p1/2	3.011(-1)	2.525(-1)	1.636(-1)	1.202(-1)	8.288(-2)	6.980(-2)	5.392(-2)	3.724(-2)
-3p3/2	6.035(-1)	5.081(-1)	3.369(-1)	2.591(-1)	2.060(-1)	1.965(-1)	2.079(-1)	2.786(-1)
-4p1/2	3.948(-4)	1.303(-2)	5.417(-2)	7.905(-2)	1.023(-1)	1.109(-1)	1.213(-1)	1.323(-1)
-4p3/2	7.229(-4)	2.532(-2)	1.042(-1)	1.489(-1)	1.830(-1)	1.903(-1)	1.866(-1)	1.519(-1)
-5p1/2	6.756(-4)	5.998(-3)	1.825(-2)	2.429(-2)	2.935(-2)	3.106(-2)	3.300(-1)	3.476(-2)
-5p3/2	1.301(-3)	1.174(-2)	3.546(-2)	4.651(-2)	5.429(-2)	5.590(-2)	5.518(-2)	4.766(-2)
4s1/2-4p1/2	4.631(-1)	3.880(-1)	2.470(-1)	1.793(-1)	1.226(-1)	1.030(-1)	8.006(-2)	5.470(-2)
-4p3/2	9.277(-1)	7.802(-1)	5.078(-1)	3.855(-1)	3.028(-1)	2.873(-1)	3.027(-1)	4.009(-1)
-5p1/2	3.039(-4)	8.319(-3)	5.278(-2)	8.177(-2)	1.100(-1)	1.203(-1)	1.325(-1)	1.460(-1)
-5p3/2	6.760(-4)	1.597(-2)	1.009(-1)	1.526(-1)	1.938(-1)	2.025(-1)	1.971(-1)	1.558(-1)
5s1/2-5p1/2	6.072(-1)	5.091(-1)	3.224(-1)	2.339(-1)	1.592(-1)	1.335(-1)	1.042(-1)	7.105(-2)
-5p3/2	1.216	1.023(-1)	6.625(-1)	5.024(-1)	3.921(-1)	3.715(-1)	3.914(-1)	5.164(-1)
3p1/2-4s1/2	1.503(-1)	1.198(-1)	8.055(-2)	6.511(-2)	5.345(-2)	4.964(-2)	4.530(-2)	4.053(-2)
-5s1/2	1.868(-2)	1.899(-2)	1.550(-2)	1.328(-2)	1.139(-2)	1.072(-2)	9.935(-3)	9.038(-3)
3p3/2-4s1/2	1.508(-1)	1.207(-1)	8.262(-2)	6.866(-2)	6.034(-2)	5.914(-2)	6.175(-2)	7.543(-2)
-5s1/2	1.870(-2)	1.907(-2)	1.579(-2)	1.384(-2)	1.254(-2)	1.233(-2)	1.271(-2)	1.472(-2)
4p1/2-5s1/2	2.687(-1)	2.075(-1)	1.345(-1)	1.075(-1)	8.773(-2)	8.135(-2)	7.430(-2)	6.620(-2)
4p3/2-5s1/2	2.694(-1)	2.089(-1)	1.377(-1)	1.130(-1)	9.847(-2)	9.614(-2)	9.989(-2)	1.202(-1)

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