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Breit-Pauli Approximation for Highly Ionized Beryllium-like
Ions Kr XXXIII, Mo XXXIX and W LXXI.

by

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Abstract: We have calculated oscillator strengths and transition probabilities for transitions between the $1s^2 2s^2$, $1s^2 2s 2p$ and $1s^2 2p^2$ states, namely: $1s^e_0 \rightarrow 1p^0_1$; $1p^0_1 \rightarrow 1d^e_2$; $1p^0_1 \rightarrow 1s^e_0$ and $3p^0_J \rightarrow 3p^e_J$. A common set of radial functions is used. It is found that for allowed transitions the one-electron relativistic operators are more important than the Breit-Pauli corrections.

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1. Introduction

In connection with the impurity problem and radiation cooling of high-temperature plasma accurate determination of excitation energies, oscillator strengths and transition probabilities of highly ionized atoms are required, Smith (1973), Wiese and Younger (1976), Feldman and Doschek (1977), Darwin (1978, 1979). Of these ions beryllium-like ions are particularly important.

Accurate experimental determinations of transition probabilities are difficult, Martinson et al (1974). Theoretical calculations for the $2s^2 1S_0^e \rightarrow 2s 2p 1P_0^0$ transition for beryllium-like ions have been made recently by Kim and Desclaux (1976) and by Armstrong et al (1976) using the relativistic multiconfigurational Hartree-Fock method. The relativistic random-phase-approximation methods have also been used by Lin and Johnson (1977) and by Cheng and Johnson (1977) to calculate oscillator strengths in the beryllium sequence.

The present investigation extends these studies by considering absorption transitions of allowed transitions between the $n = 2$ states for Kr XXXIII, Mo XXXIX and W LXXI. These ions were chosen for their importance in studies of controlled thermonuclear reactions.

2. Radial Functions

The radial functions used in the calculations were determined in an LS-coupled representation of the atomic states. The atomic-state wavefunctions are represented by the configuration interaction expansion

$$\Psi(LS) = \sum_{i=1}^{M_s} a_i \phi(\alpha_i:LS) \quad (1)$$

where L and S are the total orbital and spin angular momenta, and α_i specifies the angular momentum coupling scheme of the i th configuration. The configurational wavefunctions $\{\phi_i\}$ are constructed

according to $\{\alpha_i\}$ from the one-electron functions

$$u_{n\ell m_\ell}(\underline{r}, m_s) = \frac{1}{r} P_{n\ell}(r) Y_\ell^{m_\ell}(\theta, \phi) \chi(m_s) \quad (2)$$

where the radial functions $\{P_{n\ell}; n = \ell + 1, \dots\}$ form an orthonormal set. We have chosen to express these in terms of Slater-type-orbitals (STO)

$$P_{n\ell}(r) = \sum_{j=1}^k C_{jn\ell} r^{I_{jn\ell}} \exp(-\zeta_{jn\ell} r) \quad (3)$$

where

$$k \geq n - \ell \quad (4)$$

The coefficients $\{a_i\}$ in (1) are, for a given set of $\{\phi_i\}$, the components of the appropriate eigenvector of the Hamiltonian matrix with element

$$H_{ij} = \langle \phi_i | \mathcal{H} | \phi_j \rangle \quad (5)$$

where $\mathcal{H}$ represents the non-relativistic Hamiltonian operator. The corresponding eigenvalue E is given by

$$E = \langle \Phi | \mathcal{H} | \Phi \rangle \quad (6)$$

where Φ is normalized to unity and E is an upper bound to the corresponding exact energy (MacDonald 1933)

$$E \geq E_{\text{exact}} \quad (7)$$

Different choices of the parameters $C_{jn\ell}$; $I_{jn\ell}$; $\zeta_{jn\ell}$ in (3) subject to the orthonormality condition, will lead to different functions $\{\phi_i\}$ and hence to different values of E and $\{a_i\}$. The upper-bound property (7) may then be used to determine optimal values of the parameters in (3).

We chose the 1s, 2s and 2p functions as the Hartree-Fock (HF) functions of the $2s\ 2p\ ^1P^0$ state. The HF functions were determined

approximately (i.e. without an SCF procedure) using CIV3 (Hibbert 1975, Glass and Hibbert 1979). In earlier calculations of allowed transitions (Hibbert 1974, Glass 1979a) it was found that, except where cancellations were severe, a reasonably accurate transition probability could be obtained by using 3s, 3p, 3d and 4f correlation orbitals and by including all possible configurations keeping a $1s^2$ core. As a starting point, we adopt the same procedure here. The 3s, 3p, 3d and 4f functions were optimized on the seven possible configurations of $1D^e$:

$$2p^2; 2p\ 3p; 3p^2; 2s\ 3d; 3s\ 3d; 3d^2; 2p\ 4f.$$

In obtaining the correlation orbitals, we have chosen

$$k = n - l \quad (8)$$

so that the coefficients $\{C_{jnl}\}$ are uniquely determined by the orthogonality conditions for a specified basis set of Slater-type orbitals.

The values of $\{I_{jnl}\}$ have been taken to satisfy

$$I_{1nl} = l + 1 \quad (9)$$

$$I_{j+1,nl} = I_{jnl} + 1 \quad (j \geq 1)$$

The coefficients and exponents of the HF functions are given in table 1.

The correlation orbitals exponents are given in table 2.

3. Results and Discussion

In table 3 a list of configurations for each state is given. The first six wavefunctions are LS coupled and are used in the expansions for the last ten intermediate-coupled wavefunctions. The eigenvector for each intermediate-coupled eigenstate are given together with corresponding eigenvalue in tables 4-6. The ordering is given by table 3. In obtaining the eigenvectors in calculation a: the one-electron relativistic operators were included in

the Hamiltonian, while in calculation b: the spin-other-orbit and spin-spin interactions were also included. We have also used the definition of spherical harmonics given by Fano and Racah (1959) which includes a factor of i^l to give time-reversal invariance.

From our earlier work (Glass 1979a) on the beryllium sequence, $12 \leq Z \leq 26$, we found that including the spin-other-orbit and spin-spin interactions in the Hamiltonian had little or no effect on energy levels of intermediate-coupled eigenstates. From tables 4-6 it is seen that a similar situation also exists for Kr XXXIII, Mo XXXIX and W LXXI. Also from tables 4-6 it is seen that, except where states of the same J-value cross, there is a "stronger" mixing between different states of a particular J-level when spin-other-orbit and spin-spin interactions are omitted. Where crossing occurs between states of the same J-value there is a "stronger" mixing between these states when the Breit-Pauli corrections are included in the Hamiltonian. A similar situation also exists in the boron sequence where $2s^2 2p^2 P^0$ and $2s 2p^2 S^e$, $J = 1/2$, levels cross (Glass 1979b).

From table 4 we see that the $2p^2 3P^e$ and $2p^2 1D^e$, $J = 2$ levels show a crossing near krypton. The $2s 2p^1 P^0$ and $2p^2 3P^e$, $J = 0$ levels also show a crossing in the neighborhood of krypton, tables 4 and 5. And from tables 5 and 6 it is seen that the $2s 2p^3 P^0$ and $2p^2 3P^e$, $J = 0$ levels show a crossing in the neighborhood of molybdenum.

Calculated energy differences between ground state and each excited states are given in table 7. It is seen that energy differences calculated using the simpler calculation a: (including only the one-electron relativistic operators in the Hamiltonian) are in very good agreement with calculation b: where spin-other-orbit and spin-spin interactions are also included in the Hamiltonian.

In tables 7-12 we present our results for the corresponding oscillator strengths, theoretical values of $\{\Delta E\}$, the energy difference of the two states in a transition, wavelength $\{\lambda\}$ and transition probabilities $\{A\}$ calculated using the length form. The agreement between length and velocity forms using HF functions is poor, calculation a: of tables 7-12. However, excellent agreement can be obtained by including in the CI expansion all possible configurations which can be formed using $1s$, $2s$, $2p$, $3s$, $3p$, $3d$ and $4f$ functions keeping the $1s^2$ core unchanged, calculation b: of tables 7-12, with the length value becoming seemingly rather more stable.

We next considered the effect of including the one-electron J-independent relativistic operators in the Hamiltonian. Calculation c: of tables 7-12 represents results obtained using only HF functions, while calculation d: represents results obtained using the CI expansions. Comparing calculations c: and d: we see that the energy difference $\{\Delta E\}$ and oscillator strengths (length form) changes, increasing rapidly with increasing Z , when the CI expansions are used.

The next stage of our investigation was to include the J-dependent terms, nuclear spin-orbit, spin-other-orbit and spin-spin interactions, in the Hamiltonian as well as one-electron non-fine structure operators. We first considered the effect of including the nuclear spin-orbit interaction in the Hamiltonian, calculation e: of tables 7-12. The energy difference $\{\Delta E\}$ for the $2s^2 1S_0^e \rightarrow 2s 2p 1P_1^0$ and $2s 2p 1P_1^0 \rightarrow 2p^2 1S_0^e$ transitions are increased. When J-dependent terms are introduced into the Hamiltonian interaction between different LS states of the same J-value are included by way of the spin-orbit interaction. This results in the energy of a state being lowered or raised. For example, including the $2p^2 3P_0^e$ configuration in the $2s^2 1S_0^e$ CI expansion, lowers the energy of the $2s^2 1S_0^e$ state of krypton by 0.02 au. while including the $2s 2p 3P_1^0$

configuration in the $2s\ 2p\ ^1P_1^0$ CI expansion the energy of the $2s\ 2p\ ^1P_1^0$ state is raised by 0.42 au. It is interesting that; although, the energy difference $\{\Delta E\}$ for the $2s^2\ ^1S_0 \rightarrow 2s\ 2p\ ^1P_1^0$ transition is increased, the oscillator strength is decreased. This is due to the change in magnitude of the $2s^2\ ^1S_0$ and $2s\ 2p\ ^1P_1^0$ coefficients when the spin-orbit interaction is included. For krypton the coefficient changes from 0.9837 and 0.9981 to 0.9804 and 0.0373 respectively.

For the $2s\ 2p\ ^1P_1^0 \rightarrow 2p^2\ ^1D_2^e$ transition, the energy difference $\{\Delta E\}$ is reduced almost by a factor of two, calculation e: of table 9, when the nuclear spin-orbit-interaction is included in the Hamiltonian. Including $2p^2\ ^3P_2^e$ configuration in the $2p^2\ ^1D_2^e$ CI expansion results in a "strong" mixing of the two configurations. The resulting interaction between the two states by way of the spin-orbit interaction lowers the energy of the $2p^2\ ^1D_2^e$ state by 1.13 au for krypton. The oscillator strength is changed by a factor of 5 (krypton) when the nuclear spin-orbit interaction is included. This is due to (i) a decrease in the energy difference $\{\Delta E\}$, (ii) including $2p^2\ ^3P_2^e$ configuration in the $2p^2\ ^1D_2^e$ CI expansion changes the coefficient of the $2p^2\ ^1D_2^e$ configuration from 0.9996 to 0.7290 and (iii) the contribution from the matrix element, $\langle 2s\ 2p\ ^3P_1^0 | \sum_i \mathbf{r}_i | 2p^2\ ^3P_2^e \rangle$, results in a large cancellation of the oscillator strength.

For the multiplet transition $2s\ 2p\ ^3P^0 \rightarrow 2p^2\ ^3P^e$ we found (Glass 1979a) that the oscillator strength determined by including the one-electron J-independent relativistic operators in the Hamiltonian were in quite good agreement with the weighted multiplet oscillator strengths $\sum_{JJ'} gf(J - J')$ where g is the statistical weight of the initial state and $f(J - J')$ the oscillator strength (length form) for the transition, $2s\ 2p\ ^3P_J^0 \rightarrow 2p^2\ ^3P_J^e$. However, from tables 10-12 we see that for Kr XXXIII, Mo XXXIX and W LXXI the agreement is disappointing. For example for krypton they differ by approximately

33%, an indication of the growth of the intercombination and forbidden transitions which becomes significant somewhere between Fe XXIII and Kr XXXIII.

We repeated the calculations including the spin-other-orbit and spin-spin interactions in the Hamiltonian, calculation f: tables 7-12. As in our earlier work (Glass 1979a, b, c, d) we see that quite accurate calculations of energy differences between states, oscillator strengths and transition probabilities can be obtained without including spin-other-orbit and spin-spin interactions in the Hamiltonian. Since calculations including Breit-Pauli correction are fairly time-consuming this is very important.

Our results, for transitions between $2s^2 1S_0^e$ and $2s 2p 1P_1^0$ states, are in very good agreement with other theoretical results. For Kr XXXIII and Mo XXXIX agreement with theoretical calculation of Armstrong et al (1976), calculation h: of table 7, who used the relativistic multiconfigurational Hartree-Fock method, and the relativistic random-phase-approximation method used by Lin and Johnson (1977), calculation i: of table 7, is excellent. For W LXXI our results for the oscillator strength is about 10% higher than those of Armstrong et al (1976). For the energy separation of the two states they obtain a value of 64.78 au. If we exclude the J-dependent operators we obtain a value 67.07 au; including the J-dependent terms the value changes to 84.87 au. Comparing our values for the transition probabilities of Kr XXXIII and Mo XXXIII with those of Weiss (1976), calculation g: of table 7, for molybdenum agreement is very good, whereas agreement for krypton is disappointing. Weiss value for the transition probability for krypton is in very good agreement with our value obtained by only including the non-fine structure terms in the Hamiltonian.

We have presented in this paper some fairly extensive CI calculations of energy difference, oscillator strengths, wavelengths and transition

probabilities for Kr XXXIII, Mo XXXIX and W LXXI. For the lower members of the sequence, Ca XVII and Fe XXIII we (Glass 1979a) found that for multiplet transitions and transitions between singlet states, quite accurate results for oscillator strengths, transition probabilities and energy differences between states could be obtained by including, in addition to the non-relativistic terms, the one-electron J-independent relativistic operators in the Hamiltonian. However, for $Z > 26$ we see that this is no longer a valid statement. For allowed transitions we found that, also including the nuclear spin-orbit interaction in the Hamiltonian, quite accurate calculations of energy differences between states, oscillator strengths and transition probabilities between different J states could be obtained. We see that this is also the case for Kr XXXIII, Mo XXXIX and W LXXI. Unfortunately there are no theoretical results for us to compare our results for transitions between the $2s\ 2p$ and $2p^2$ states with.

Acknowledgement

This work was supported by the U.S. Department of Energy under contract number EG-77-S-02-4264.

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Table 1. Hartree-Fock function parameters.

nl	I_{jnl}	Kr XXXIII	Mo XXXIX	W LXXI
		ζ_{jnl}		
1s	1	35.78038	41.64841	73.80057
1s	1	64.00064	70.24221	129.51143
2s	2	16.75315	19.77185	35.69331
2s	2	22.58243	26.59388	47.67476
2s	2	30.99293	36.98309	65.60974
2p	2	16.44842	19.43960	35.35576
2p	2	18.56537	21.56758	37.42062
2p	2	27.25258	31.15496	53.96017
2p	2	75.00989	90.33333	158.93752
		C_{jnl}		
1s		0.98191	0.98444	0.99012
		0.00690	0.00863	0.00372
		0.00298	0.00228	0.00147
		-0.00304	-0.00098	-0.00129
		0.01570	0.00905	0.00826
2s		-0.33721	-0.33910	-0.34515
		-0.00013	-0.00111	-0.00024
		1.42147	1.45096	1.48521
		-0.25229	-0.29800	-0.32492
		-0.18596	-0.16893	-0.17637
2p		0.78219	0.78965	0.76977
		0.20063	0.19188	0.21544
		0.02134	0.02200	0.01673
		0.00023	0.00019	0.00011

Table 2. Correlation orbital exponents.

$n\ell$	$I_{jn\ell}$	Kr XXXIII	Mo XXXIX	W LXXI
		$\zeta_{jn\ell}$		
3s	1	15.84076	18.80080	33.32574
	2	15.89143	18.68067	33.60180
	3	15.88009	18.67329	33.54763
3p	2	18.15614	18.02384	31.50651
	3	18.14877	20.98905	37.31945
3d	3	19.19153	22.62167	40.85473
4f	4	24.67002	29.02242	52.22402

Table 3. Configurations used for each state.

$\Psi(2s^2 1s^e)$	$[1s^2] 2s^2, 2p^2, 2s 3s, 3s^2, 2p 3p, 3p^2, 3d^2$
$\Psi(2s 2p 3p^0)$	$[1s^2] 2s 2p, 2s 3p, 3s 2p, 3s 3p, 2p 3d, 3p 3d, 3d 4f$
$\Psi(2s 2p 1p^0)$	$[1s^2] 2s 2p, 2s 3p, 3s 2p, 3s 3p, 2p 3d, 3p 3d, 3d 4f$
$\Psi(2p^2 3p^e)$	$[1s^2] 2p^2, 2p 3p, 3p^2, 3d^2$
$\Psi(2p^2 1D^e)$	$[1s^2] 2p^2, 2p 3p, 3p^2, 2s 3d, 3s 3d, 3d^2, 2p 4f, 3p 4f$
$\Psi(2p^2 1s^e)$	$[1s^2] 2s^2, 2p^2, 2s 3s, 3s^2, 2p 3p, 3p^2, 3d^2$
$\Psi(2s^2 1s_0^e)$	$\Psi(2s^2 1s_0^e), \Psi(2p^2 3p_0^e)$
$\Psi(2s 2p 3p_0^0)$	$\Psi(2s 2p 3p_0^0)$
$\Psi(2s 2p 3p_1^0)$	$\Psi(2s 2p 3p_1^0), (2s 2p 1p_1^0)$
$\Psi(2s 2p 3p_2^0)$	$\Psi(2s 2p 3p_2^0)$
$\Psi(2s 2p 1p_1^0)$	$\Psi(2s 2p 1p_1^0), \Psi(2s 2p 3p_1^0)$
$\Psi(2p^2 3p_0^e)$	$\Psi(2p^2 3p_0^e), \Psi(2s^2 1s_0^e)$
$\Psi(2p^2 3p_1^e)$	$\Psi(2p^2 3p_1^e)$
$\Psi(2p^2 3p_2^e)$	$\Psi(2p^2 3p_2^e), \Psi(2p^2 1D_2^e)$
$\Psi(2p^2 1D_2^e)$	$\Psi(2p^2 1D_2^e), \Psi(2p^2 3p_2^e)$
$\Psi(2p^2 1s_0^e)$	$\Psi(2p^2 1s_0^e), \Psi(2p^2 3p_0^e)$

Table 4. Eigenvalues and eigenvectors for Kr XXXIII. (All energies in atomic units).

	$2s^2 1s_0^e$	$2s. 2p^3 p_0^0$	$2s 2p^3 p_1^0$	$2s 2p^3 p_2^0$	$2s 2p^1 p_1^0$	$2p^2 3p_0^e$	$2p^2 3p_1^e$	$2p^2 1d_2^e$	$2p^2 3p_2^e$	$2p^2 1s_0^e$
Calculation a: E	-1592.63872	-1590.35328	-1589.93614	-1587.75801	-1586.11928	-1586.07637	-1584.01325	-1583.59539	-1581.20583	-1579.97049
{a ₁ }	0.9804	0.9974	0.3416	0.9981	0.9377	-0.1209	-0.9995	-0.6837	0.7295	0.1307
	-0.1701	0.0383	0.0205	0.0085	0.1531	-0.4218	-0.0316	-0.0193	0.0063	0.8900
	-0.0841	0.0004	-0.0184	0.0021	-0.0511	0.0068	0.0027	0.0019	-0.0022	-0.0039
	0.0009	0.0601	0.0001	0.0603	0.0027	0.0012	0.0051	0.0035	-0.0038	-0.0027
	-0.0014	-0.0067	-0.0065	-0.0069	-0.0182	-0.0267		0.7290	0.6838	0.0103
	-0.0005	0.0010	0.0002	0.0009	0.0008	0.0020		0.0234	0.0086	-0.0054
	-0.0031	-0.0010	-0.0013	0.0010	-0.0035	0.0051		-0.0027	-0.0028	-0.0104
	-0.0525		0.9372		-0.3422	-0.8971		-0.0111	-0.0107	-0.4365
	-0.0051		0.0316		0.0038	-0.0434		0.0024	0.0023	0.0008
	0.0001		0.0007		-0.0010	0.0018		-0.0037	-0.0035	0.0014
	0.0002		0.0565		-0.0208	0.0046		-0.0033	-0.0031	0.0022
			0.0064		0.0023			-0.0002	-0.0002	
			0.0009		-0.0004					
			-0.0010		0.0003					
Calculation b: E	-1592.63515	-1590.21651	-1589.82685	-1587.81777	-1586.16273	-1585.82843	-1583.93289	-1583.55175	-1581.32091	-1580.06748
{a ₁ }	0.9810	0.9975	0.3301	0.9981	-0.9418	-0.1142	-0.9995	-0.6941	0.7196	0.1323
	-0.1683	0.0370	0.0195	0.0091	-0.0158	-0.4155	-0.0310	-0.0194	0.0069	0.8933
	-0.0841	0.0005	-0.0178	0.0021	0.0513	-0.0062	0.0027	0.0019	-0.0022	-0.0041
	0.0009	0.0601	0.0001	0.0604	-0.0027	0.0012	0.0052	0.0035	-0.0037	0.0027
	-0.0012	-0.0068	-0.0062	-0.0070	0.0183	-0.0255		0.7191	0.6942	0.0111
	-0.0005	0.0010	0.0002	0.0009	-0.0008	0.0020		0.0228	0.0094	-0.0054
	-0.0031	-0.0010	-0.0012	-0.0010	0.0035	0.0050		-0.0027	-0.0029	-0.0105
	-0.0471		0.9413		0.3306	-0.9010		-0.0110	-0.0109	-0.4292
	-0.0046		0.0306		-0.0035	-0.0419		0.0024	0.0023	0.0005
	0.0000		0.0007		0.0010	0.0019		-0.0037	-0.0035	0.0014
	0.0002		0.0567		0.0201	0.0046		-0.0032	-0.0031	0.0022
			-0.0064		-0.0022			-0.0002	-0.0002	
			0.0009		0.0004					
			-0.0009		-0.0003					

Table 4 Continued

- a: CI (Non-relativistic + one-electron mass correction + one-electron Darwin contact term + nuclear spin-orbit interaction)
- b: CI (Non-relativistic + one-electron mass correction + one-electron Darwin contact term + nuclear spin-orbit + spin-other-orbit + spin-spin interaction)

Table 5. Eigenvalues and eigenvectors for Mo XXXIX. (All energies in atomic units).

	$2s^2 1s_e^0$	$2s 2p^3 p_0^0$	$2s 2p^3 p_1^0$	$2s 2p^3 p_2^0$	$2p^2 3p_e^0$	$2s 2p^1 p_1^0$	$2p^2 3p_e^1$	$2p^2 1d_e^2$	$2p^2 3p_e^2$	$2p^2 1s_e^0$
Calculation a: E	-2193.12831	-2190.31257	-2189.72266	-2185.22683	-2185.01895	-2183.37835	-2180.55342	-2180.03161	-2175.32735	-2173.96055
{a _i }	0.9801	0.9951	0.4153	0.9965	-0.1288	0.9056	-0.9989	-0.6423	0.7658	-0.0988
	-0.1491	0.0551	0.0302	0.0134	-0.4752	0.0190	-0.0470	-0.0283	0.0127	-0.8659
	-0.1138	-0.0022	-0.0318	0.0011	0.0116	-0.0698	0.0016	0.0011	-0.0019	0.0056
	0.0042	0.0815	-0.0011	0.0818	0.0008	0.0014	0.0043	0.0028	-0.0034	0.0020
	-0.0041	-0.0057	-0.0067	-0.0059	-0.0406	-0.0150		0.7650	0.6427	-0.0167
	-0.0006	0.0008	0.0002	0.0008	0.0010	0.0006		0.0363	0.0129	0.0042
	-0.0028	-0.0009	-0.0013	-0.0009	0.0048	-0.0029		-0.0019	-0.0021	0.0085
	-0.0648		0.9044		-0.8671	-0.4163		-0.0099	-0.0086	0.4899
	-0.0075		0.0458		-0.0632	0.0010		0.0023	0.0019	0.0040
	-0.0001		-0.0016		0.0001	-0.0009		-0.0033	-0.0028	-0.0013
	0.0002		0.0740		0.0037	-0.0343		-0.0029	-0.0025	-0.0021
			-0.0053			0.0023		-0.0002	-0.0001	
			0.0007			-0.0004				
			-0.0008			0.0004				
Calculation b: E	-2193.12148	-2190.08046	-2189.52572	-2185.32532	-2184.58834	-2183.46031	-2180.41873	-2179.95298	-2175.52234	-2174.12892
{a _i }	0.9809	0.9952	0.4073	0.9965	-0.1211	0.9092	-0.9989	-0.6489	0.7602	0.0999
	-0.1461	0.0535	0.0291	0.0141	-0.4727	0.0197	-0.0463	-0.0283	0.0134	0.8679
	-0.1139	-0.0020	-0.0311	0.0011	0.0107	-0.0701	0.0017	0.0011	-0.0018	-0.0057
	0.0042	0.0814	-0.0010	0.0818	0.0008	0.0014	0.0044	0.0028	-0.0033	-0.0020
	-0.0037	-0.0057	-0.0065	-0.0059	-0.0392	-0.0151		0.7594	0.6493	0.0176
	-0.0006	0.0008	0.0002	0.0007	0.0011	0.0006		0.0357	0.0137	-0.0042
	-0.0028	-0.0009	-0.0013	-0.0009	0.0048	-0.0029		-0.0019	-0.0022	-0.0085
	-0.0579		0.9082		-0.8697	-0.4082		-0.0098	-0.0087	-0.4862
	-0.0068		0.0446		-0.0614	0.0007		0.0023	0.0020	-0.0044
	-0.0001		-0.0015		0.0002	-0.0009		-0.0033	-0.0028	0.0013
	0.0002		0.0743		0.0038	-0.0336		-0.0029	-0.0025	0.0021
			-0.0053			0.0023		-0.0002	-0.0002	
			0.0007			-0.0004				
			-0.0008			0.0003				

Table 5 Continued

- a: CI (Non-relativistic + one-electron mass correction + one-electron Darwin contact term + nuclear spin-orbit interaction)
- b: CI (Non-relativistic + one-electron mass correction + one-electron Darwin contact term + nuclear spin-orbit + spin-other-orbit + spin-spin interaction)

Table 6. Eigenvalues and eigenvectors for W LXXI. (All energies in atomic units).

	$2s^2 1s_e^0$	$2s 2p^3 p_0^0$	$2s 2p^3 p_1^0$	$2p^2 3p_e^0$	$2s 2p^3 p_2^0$	$2s 2p^1 p_1^0$	$2p^2 3p_e^1$	$2p^2 1d_e^2$	$2p^2 3p_e^2$	$2p^2 1s_e^0$
Calculation a: E	-7302.43709	-7288.68398	-7287.24663	-7269.65259	-7220.17171	-7216.94988	-7195.84946	-7194.74061	-7133.79804	-7131.59442
{a _i }	0.9136	0.9331	0.5146	0.0629	0.9553	-0.7964	-0.9816	-0.5768	0.8067	0.0191
	-0.0531	0.2126	0.1219	0.5350	0.0552	-0.0500	-0.1901	-0.1106	0.0650	0.8217
	-0.3918	-0.0632	-0.1548	-0.0253	-0.0156	0.2405	-0.0167	-0.0096	0.0013	-0.0062
	0.0829	0.2830	-0.0359	0.0045	0.2900	0.0136	0.0023	0.0014	-0.0020	0.0000
	-0.0120	-0.0027	-0.0043	0.1735	-0.0032	0.0074		0.7944	0.5854	0.0674
	-0.0022	0.0002	-0.0004	0.0262	0.0001	0.0003		0.1538	0.0484	0.0003
	-0.0019	-0.0004	-0.0009	-0.0026	-0.0005	0.0015		0.0130	0.0007	-0.0044
	-0.0425		0.7785	0.7838		0.5279		-0.0058	-0.0051	-0.5638
	-0.0154		0.1749	0.2501		0.0257		-0.0023	0.0018	-0.0429
	-0.0024		-0.0519	0.0386		-0.0073		-0.0019	-0.0014	-0.0006
	0.0001		0.2360	-0.0018		0.1604		-0.0017	0.0014	0.0013
			-0.0024			-0.0015		-0.0003	-0.0002	
			0.0001			0.0002				
			-0.0004			-0.0003				
E	-7302.42045	-7286.74486	-7285.51319	-7265.93678	-7220.82440	-7217.54765	-7194.83804	-7194.12409	-7135.09907	-7132.72347
{a _i }	0.9140	0.9340	0.5142	-0.0562	0.9552	-0.7969	-0.9819	-0.5787	0.8052	-0.0192
	-0.0495	0.2093	0.1200	-0.5367	0.0565	-0.0512	-0.1885	-0.1104	0.0667	-0.8213
	-0.3920	-0.0620	-0.1546	0.0223	-0.0161	0.2407	-0.0163	-0.0096	0.0015	0.0063
	0.0829	0.2829	-0.0353	-0.0039	0.2900	0.0139	0.0024	0.0013	-0.0019	-0.0000
	-0.0106	-0.0026	-0.0043	-0.1710	-0.0032	0.0074		0.7932	0.5871	-0.0690
	-0.0019	0.0003	-0.0003	-0.0254	0.0000	0.0004		0.1528	0.0499	-0.0005
	-0.0019	-0.0005	-0.0009	0.0026	-0.0005	0.0014		0.0129	0.0008	0.0044
	-0.0366		0.7797	-0.7851		0.5270		-0.0058	-0.0051	0.5643
	-0.0132		0.1724	-0.2462		0.0264		0.0023	0.0018	0.0439
	-0.0021		-0.0512	-0.0372		-0.0075		-0.0019	-0.0014	0.0005
	0.0000		0.2362	0.0019		0.1601		-0.0017	-0.0014	-0.0013
			-0.0023			-0.0014		-0.0003	-0.0002	
			0.0001			0.0002				
			-0.0004			-0.0002				

Table 6 Continued

- a: CI (Non-relativistic + one-electron mass correction + one-electron Darwin contact term + nuclear spin-orbit interaction)
- b: CI (Non-relativistic + one-electron mass correction + one-electron Darwin contact term + nuclear spin-orbit + spin-other-orbit + spin-spin interaction)

Table 7. Excitation thresholds (in au) for Kr XXXIII, Mo XXXIX and W LXXI.

	Kr XXXIII		Mo XXXIX		W LXXI	
	Calculation a:	Calculation b:	Calculation a:	Calculation b:	Calculation a:	Calculation b:
$2s^2 1s_0^e$	0.0	0.0	0.0	0.0	0.0	0.0
$2s 2p^3 p_0^0$	2.28544	2.41864	2.81574	3.04102	13.75311	15.67559
$2s 2p^3 p_1^0$	2.70258	2.8083	3.40565	3.59576	15.19046	16.09726
$2s 2p^3 p_2^0$	4.88071	4.81738	7.90148	7.79616	32.7845 [†]	36.48367 [†]
$2s 2p^1 p_1^0$	6.51944	6.47242	8.10936 [*]	8.53314 [*]	82.26538 [†]	81.59605 [†]
$2p^2 3p_0^e$	6.56235	6.80672	9.74996 [*]	9.66117 [*]	85.48721 [†]	84.8728 [†]
$2p^2 3p_1^e$	8.62547	8.70226	12.57489	12.70275	106.58763	107.58241
$2p^2 1d_2^e$	9.04333	9.0834	13.0967	13.1685	107.69648	108.29636
$2p^2 3p_2^e$	11.43289	11.31424	17.80096	17.59914	168.63905	167.32138
$2p^2 1s_0^e$	12.66823	12.56767	19.16776	18.99256	170.84267	169.69638

a: CI (Non-relativistic + one-electron mass correction + one-electron Darwin contact term + nuclear spin-orbit interaction)

b: CI (Non-relativistic + one-electron mass correction + one-electron Darwin contact term + nuclear spin-orbit + spin-other-orbit + spin-spin interaction)

* For Mo XXXIX the $2s 2p^1 p_1^0$ and $2p^2 3p_0^e$ levels are interchanged.

† For W LXXI the $2p^2 3p_0^e$ level lies below the $2s 2p^3 p_2^0$ and $2s 2p^1 p_1^0$ levels.

Table 7. Energy differences $\{\Delta E\}$, wavelengths $\{\lambda\}$, oscillator strengths $\{f\}$ and transition probabilities $\{A\}$ for allowed transition $2s^2 1S_0^e \rightarrow 2s 2p 1P^0$. (All energies in au: λ in units of $\text{\AA}$: A in units of 10^8 Sec^{-1}).

Z	Calculation	ΔE	λ	f_ℓ	f_v	A
36	a	4.2391	107.5	0.093	0.056	179.58
	b	4.2044	108.4	0.093	0.093	175.25
	c	5.7515	79.2	0.143		505.45
	d	6.0757	75.0	0.143		567.23
	e	6.5195	69.9	0.137		624.85
	f	6.4724	70.4	0.137		616.58
	g		73.2			572.0
	h	6.363		0.137		
	i			0.136		
42	a	4.9804	91.5	0.079	0.048	210.66
	b	4.9460	92.1	0.079	0.079	206.35
	c	7.8742	57.9	0.147		976.03
	d	8.6733	52.5	0.151		1217.56
	e	9.7500	46.7	0.142		1449.94
	f	9.6612	47.2	0.142		1422.15
	g		50.9			1210.0
	h	9.260		0.140		
	i			0.140		
74	a	8.9326	51.0	0.044	0.027	376.28
	b	8.8985	51.2	0.044	0.044	371.97
	c	39.4880	11.5	0.259		43248.3
	d	67.0728	6.8	0.320		154307.0
	e	85.4872	5.3	0.299		234055.0
	f	84.8728	5.4	0.297		229218.0
	h	64.78		0.265		

a: HF (Non-relativistic)

b: CI (Non-relativistic)

c: HF (Non-relativistic + one-electron mass correction + one-electron Darwin contact term)

d: CI (Non-relativistic + one-electron mass correction + one-electron Darwin contact term)

e: CI (Non-relativistic + one-electron mass correction + one-electron Darwin contact term + nuclear spin-orbit interaction)

f: CI (Non-relativistic + one-electron mass correction + one-electron Darwin contact term + nuclear spin-orbit + spin-other-orbit + spin-spin interaction)

Table 7 Continued

- g: Weiss (1976)
- h: Armstrong et al (1976)
- i: Lin and Johnson (1977)

Table 8. Energy differences $\{\Delta E\}$, wavelengths $\{\lambda\}$, oscillator strengths $\{f\}$ and transition probabilities $\{A\}$ for allowed transitions $2s\ 2p\ ^1P_1^0 \rightarrow 2p^2\ ^1S_0^e$. (All energies in au: λ in units of Å: A in units of $10^8\ \text{Sec}^{-1}$).

Z	Calculation	ΔE	λ	f_ℓ	f_v	A
36	a	3.6353	125.3	0.024	0.002	302.72
	b	3.6317	125.5	0.023	0.024	292.64
	c	5.1478	88.5	0.029		737.15
	d	5.4546	83.5	0.028		788.38
	e	6.1488	74.1	0.028		1030.96
	f	6.0953	74.8	0.028		1008.11
42	a	4.2830	106.4	0.020	0.0017	356.82
	b	4.2797	106.5	0.020	0.020	346.67
	c	7.1768	63.5	0.027		1352.84
	d	7.9300	57.5	0.026		1592.57
	e	9.4178	48.4	0.028		2417.46
	f	9.3314	48.8	0.028		2357.21
74	a	7.7353	58.9	0.011	0.0009	645.05
	b	7.7320	58.9	0.011	0.011	634.79
	c	38.2906	11.9	0.035		48861.0
	d	65.6309	6.9	0.039		163176.0
	e	85.3555	5.3	0.052		362256.0
	f	84.8242	5.4	0.051		355203.0

a: HF (Non-relativistic)

b: CI (Non-relativistic)

c: HF (Non-relativistic + one-electron mass correction + one-electron Darwin contact term)

d: CI (Non-relativistic + one-electron mass correction + one-electron Darwin contact term)

e: CI (Non-relativistic + one-electron mass correction + one-electron Darwin contact term + nuclear spin-orbit interaction)

f: CI (Non-relativistic + one-electron mass correction + one-electron Darwin contact term + nuclear spin-orbit + spin-other-orbit + spin-spin interaction)

Table 9. Energy differences $\{\Delta E\}$, wavelengths $\{\lambda\}$, oscillator strengths $\{f\}$ and transitions probabilities $\{A\}$ for allowed transition $2s\ 2p\ ^1P_1^0 \rightarrow 2p^2\ ^1D_2^e$. (All energies in au: λ in units of $\text{\AA}$: A in units of $10^8\ \text{Sec}^{-1}$).

Z	Calculation	ΔE	λ	f_ℓ	f_v	A
36	a	2.1434	212.6	0.037	0.051	32.92
	b	2.1462	212.3	0.036	0.033	32.30
	c	3.7804	120.5	0.066		180.64
	d	4.0765	111.8	0.065		208.60
	e	2.5239	180.5	0.013		15.74
	f	2.6110	174.5	0.013		17.21
42	a	2.5306	180.1	0.032	0.042	39.13
	b	2.5335	179.8	0.031	0.028	38.50
	c	5.6231	81.0	0.070		429.26
	d	6.3596	71.6	0.072		560.20
	e	3.3467	136.1	0.012		25.36
	f	3.5073	129.9	0.013		29.10
74	a	4.5946	99.2	0.018	0.024	72.20
	b	4.5976	99.1	0.018	0.016	71.59
	c	35.8390	12.7	0.138		34265.5
	d	62.9953	7.2	0.171		130805.0
	e	22.2093	20.5	0.015		1444.09
	f	23.4236	19.5	0.016		1690.16

a: HF (Non-relativistic)

b: CI (Non-relativistic)

c: HF (Non-relativistic + one-electron mass correction + one-electron Darwin contact term)

d: CI (Non-relativistic + one-electron mass correction + one-electron Darwin contact term)

e: CI (Non-relativistic + one-electron mass correction + one-electron Darwin contact term + nuclear spin-orbit interaction)

f: CI (Non-relativistic + one-electron mass correction + one-electron Darwin contact term + nuclear spin-orbit + spin-other-orbit + spin-spin interaction)

Table 10. Energy differences $\{\Delta E\}$, wavelengths $\{\lambda\}$, oscillator strengths $\{f\}$ and transition probabilities $\{A\}$ for allowed transitions $2s\ 2p\ ^3P_J^0 \rightarrow 2p\ ^2\ ^3P_J^e$, of Kr XXXIII. (All energies in au: λ in units of Å: A in units of $10^8\ \text{Sec}^{-1}$).

$J \rightarrow J'$	Calculation	ΔE	λ	f_ℓ	f_v	A
Multiplet	a	3.4706	131.3	0.036	0.019	139.76
	b	3.4714	131.3	0.036	0.037	138.81
	c	5.1076	89.2	0.053		445.50
	d	5.4419	83.7	0.053		504.28
$1 \rightarrow 0$	e	3.8598	118.0	0.014		195.97
	f	3.9984	114.0	0.014		215.96
	g		120.8			198.0
$1 \rightarrow 1$	e	5.9229	76.9	0.013		142.49
	f	5.8940	77.3	0.013		141.75
$1 \rightarrow 2$	e	8.7303	52.2	0.0018		25.94
	f	8.5059	53.6	0.0018		24.52
$2 \rightarrow 1$	e	3.7448	121.7	0.0091		67.98
	f	3.8849	117.3	0.0094		75.95
$2 \rightarrow 2$	e	6.5522	69.5	0.026		356.65
	f	6.4969	70.1	0.025		338.01
$0 \rightarrow 1$	e	6.3400	71.9	0.061		264.05
	f	6.2836	72.5	0.061		257.23

a: HF (Non-relativistic)

b: CI (Non-relativistic)

c: HF (Non-relativistic + one-electron mass correction + one-electron Darwin contact term)

d: CI (Non-relativistic + one-electron mass correction + one-electron Darwin contact term)

e: CI (Non-relativistic + one-electron mass correction + one-electron Darwin contact term + nuclear spin-orbit interaction)

f: CI (Non-relativistic + one-electron mass correction + one-electron Darwin contact term + nuclear spin-orbit + spin-other-orbit + spin-spin interaction)

g: Weiss (1976)

Table 11. Energy differences $\{\Delta E\}$, wavelengths $\{\lambda\}$, oscillator strengths $\{f\}$ and transition probabilities $\{A\}$ for allowed transitions $2s\ 2p\ ^3P_J^0 \rightarrow 2p^2\ ^3P_J^e$ of Mo XXXIX. (All energies in au: λ in units of Å: A in units of $10^8\ \text{Sec}^{-1}$).

$J \rightarrow J'$	Calculation	ΔE	λ	f_ℓ	f_v	A
Multiplet	a	4.0830	111.6	0.031	0.016	164.33
	b	4.0837	111.6	0.031	0.032	163.38
	c	7.1755	63.5	0.054		891.96
	d	7.9737	57.1	0.055		1119.57
$1 \rightarrow 0$	e	4.7037	96.9	0.012		257.61
	f	4.9374	92.3	0.013		295.03
	g		101.5			252.0
$1 \rightarrow 1$	e	9.1692	49.7	0.013		348.09
	f	9.1070	50.0	0.013		344.11
$1 \rightarrow 2$	e	14.3953	31.7	0.0011		45.19
	f	14.0034	32.5	0.0011		42.94
$2 \rightarrow 1$	e	4.6734	97.5	0.0080		92.99
	f	4.9066	92.9	0.0084		107.69
$2 \rightarrow 2$	e	9.8995	46.0	0.031		961.09
	f	9.8030	46.5	0.030		918.70
$0 \rightarrow 1$	e	9.7592	46.7	0.066		677.81
	f	9.6617	47.2	0.066		658.23

a: HF (Non-relativistic)

b: CI (Non-relativistic)

c: HF (Non-relativistic + one-electron mass correction + one-electron Darwin contact term)

d: CI (Non-relativistic + one-electron mass correction + one-electron Darwin contact term)

e: CI (Non-relativistic + one-electron mass correction + one-electron Darwin contact term + nuclear spin-orbit interaction)

f: CI (Non-relativistic + one-electron mass correction + one-electron Darwin contact term + nuclear spin-orbit + spin-other-orbit + spin-spin interaction)

g: Weiss (1976)

Table 12. Energy differences $\{\Delta E\}$, wavelengths $\{\lambda\}$, oscillator strengths $\{f\}$ and transition probabilities $\{A\}$ for allowed transitions $2s^2 2p^3 P_J^0 \rightarrow 2p^2 3p^1 e_{J'}$ of W LXXI. (All energies in au: λ in units of Å: A in units of 10^8 Sec^{-1}).

$J \rightarrow J'$	Calculation	ΔE	λ	f_{ℓ}	f_v	A
Multiplet	a	7.3475	62.0	0.017	0.009	295.26
	b	7.3481	62.0	0.017	0.018	294.33
	c	38.5919	11.8	0.089		42783.6
	d	66.0510	6.9	0.109		152302.0
$1 \rightarrow 0$	e	17.5940	25.9	0.0094		2802.25
	f	19.5764	23.3	0.010		3832.83
$1 \rightarrow 1$	e	91.3972	5.0	0.025		67535.5
	f	90.6751	5.0	0.025		66168.8
$1 \rightarrow 2$	e	153.4486	3.0	0.0001		462.66
	f	150.4141	3.0	0.0001		393.08
$2 \rightarrow 1$	e	24.3222	1.9	0.010		3051.37
	f	25.9864	1.8	0.010		3727.59
$2 \rightarrow 2$	e	86.3737	5.3	0.074		176450.0
	f	85.7253	5.3	0.073		171649.0
$0 \rightarrow 1$	e	92.8345	4.9	0.147		135721.0
	f	91.9068	5.0	0.146		131972.0

a: HF (Non-relativistic)

b: CI (Non-relativistic)

c: HF (Non-relativistic + one-electron mass correction + one-electron Darwin contact term)

d: CI (Non-relativistic + one-electron mass correction + one-electron Darwin contact term)

e: CI (Non-relativistic + one-electron mass correction + one-electron Darwin contact term + nuclear spin-orbit interaction)

f: CI (Non-relativistic + one-electron mass correction + one-electron Darwin contact term + nuclear spin-orbit + spin-other-orbit + spin-spin interaction)