The $2s\ 2p\ ^3P_1^0 \rightarrow 2s\ ^2\ ^1S_0$ Intercombination Line in
Beryllium-like Krypton, Molybdenum and Tungsten

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Abstract: Transition probabilities are evaluated for the $2s\ 2p\ ^3P_1^0 \rightarrow 2s\ ^2\ ^1S_0$ transition in beryllium-like ions for krypton, molybdenum and tungsten, using configuration-interaction wavefunctions. The importance of the $2s\ 3p\ ^1P_1^0$ configuration is considered.

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1. Introduction

In earlier papers (Glass and Hibbert 1978, Glass 1979a) configuration interaction (CI) wavefunctions were used to evaluate the transition probabilities for the intercombination line $2s\ 2p\ ^3P_1^0 \rightarrow 2s^2\ ^1S_0$ for beryllium-like ions for $Z = 4 - 10$, Mg IX, Si XI, Ar XV, Ca XVII and Fe XXIII. We saw that the accuracy which could be achieved for intercombination lines was not as good as that for allowed transitions, where the same level of sophistication gave results with an accuracy of over 5%. This is in part due to the fact that intercombination transition probabilities are highly sensitive to the values of the very small coefficients in the CI expansion of the wavefunctions. Also for allowed transitions quite accurate calculations of energy differences, oscillator strengths and transition probabilities could be obtained for highly ionized atoms by including the one-electron relativistic operators plus the usual non-relativistic terms in the Hamiltonian. For intercombination transitions it is also necessary to include the two body J-dependent terms (spin-other-orbit and spin-spin) in the Hamiltonian. However, from our earlier work (Glass 1979a) we saw that with increasing Z agreement between intercombination transition probabilities calculated using the simpler method (two-body J-dependent operators are omitted) and those calculated including Breit-Pauli corrections improve. For example, for Mg IX they differ by 55%, whereas for Fe XXIII they differ by 10%. Since calculations including Breit-Pauli corrections are fairly time consuming it is important to pursue the two methods further for the more highly ionized atoms of the sequence.

The way in which the radial functions are to be chosen is not as clear as for allowed transitions. For example, we optimized our np functions

on the non-relativistic $1P^0$ energy. However, one would prefer to use the relativistically coupled $J = 1$ energy, but this is dominated by the $3P_1^0$ configurations, whereas the transition probabilities depend more crucially on the relative weights of the $1P_1^0$ configurations. The transition proceeds mainly through the coupling of $3P_1^0$ and $1P_1^0$ and of $1S_0$ and $3P_0$ resulting in non-zero dipole matrix elements between $3P_1^0$ and $3P_0$ and between $1P_1^0$ and $1S_0$.

In order to perform calculations of transition probabilities, we need to determine radial functions as well as the choice of configuration and the manner in which the relativistic effects (necessary for the above coupling) are to be included. As in our previous work the radial functions will be determined variationally so as to balance the energy levels of the state involved in the transition. We shall choose configurations which correspond to all types of electron correlation: internal, semi-internal and all external.

The present investigation extends previous study by evaluating transition probabilities for the $2s\ 2p\ 3P_1^0 \rightarrow 2s^2\ 1S_0$ transition for beryllium-like ions krypton, molybdenum and tungsten. These ions were chosen for their usefulness in modeling and diagnostic studies of controlled thermonuclear reactions.

Previous theoretical values have been obtained by Armstrong et al (1976), using the relativistic multiconfigurational Hartree-Fock method, for the energy difference of the two states in the transitions and the corresponding oscillator strengths for Kr XXXIII, Mo XXXIX and W LXXI. Weiss (1976) has calculated wavelengths and transition probabilities for Kr XXXIII and Mo XXXIII. Lin and Johnson (1977) using the relativistic random-phase-approximation method have calculated the oscillator strength for the intercombination transition for Mo XXXIX.

2. Method of Calculation

2.1. *Radial functions*

The radial functions used in the final calculations were determined in an LS coupled representation of the atomic states. An LS coupled wavefunction can be written

$$\Psi(\text{LS}) = \sum_{i=1}^M a_i \Phi_i(\alpha_i; \text{LS}) \quad (1)$$

where L and S are the total orbital and spin angular momenta and $\{\alpha_i\}$ define the coupling of the angular momenta of the electrons. The radial functions $\{P_{n\ell}\}$ from which the configurational wavefunctions $\{\Phi_i\}$ are constructed were expanded in terms of Slater-type orbitals (STO)

$$P_{n\ell}(r) = \sum_{j=1}^k C_{jn\ell} r^{I_{jn\ell}} \exp(-\zeta_{jn\ell} r) \quad (2)$$

where

$$k \geq n - \ell \quad (3)$$

so that the orthonormality conditions

$$\int_0^\infty P_{n\ell}(r) P_{n'\ell}(r) dr = \delta_{nn'}, \quad (n \geq n' \geq \ell) \quad (4)$$

can be satisfied.

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

$$H_{ij} = \langle \Phi_i | H | \Phi_j \rangle \quad (5)$$

where H represents the non-relativistic Hamiltonian operator. The corresponding eigenvalues form upper bounds to the corresponding exact energies (MacDonald 1933). Different choices of the parameters $C_{jn\ell}$; $I_{jn\ell}$; $\zeta_{jn\ell}$

in (2), subject to the orthonormality condition, will lead to different functions $\{\Phi_i\}$ and hence to different values of the eigenvalue and $\{a_i\}$. The upper-bound property may then be used to determine optimal values of the parameters in (2).

We have used the general program CIV3 (Hibbert 1975, Glass and Hibbert 1979) to generate the radial functions. The 1s, 2s, and 2p functions were taken as Hartree-Fock (HF) functions of the $2s\ 2p\ 3p^0$ state. The Hartree-Fock parameters are shown in table 1.

We saw in our earlier studies (Glass and Hibbert 1978, Glass 1979a) that a reasonably accurate transition probability could be obtained using 3s, 3p, 3d, 4p and 5p orbitals and including all possible configurations keeping a $1s^2$ core. We have adopted the same procedure here. The 3s and 3d radial functions were also optimized on the $2s\ 2p\ 3p^0$ six-configuration wavefunction:

2s 2p, 2s 3p, 3s 2p, 3s 3p, 2p 3d, 3p 3d

The 3p radial function was optimized on the $2s\ 2p\ 1p^0$ six-configuration wavefunction. The 3p function was used as a correction to the 2p function for the $2s\ 2p\ 1p^0$ state. We then determined the 4p and 5p radial functions by adding configurations 2s 4p, 3s 4p, 2s 5p, 3s 5p to the $2s\ 2p\ 1p^0$ state. The exponents of the 4p and 5p functions were optimized on the $2s\ 2p\ 1p^0$ state. In obtaining the 3s, 3p, 3d, 4p and 5p radial functions we have chosen

$$k = n - \ell \quad (6)$$

so that the coefficients $\{C_{jn\ell}\}$ are uniquely determined by the orthonormality condition for a specified basis set of Slater-type orbitals.

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

$$I_{lnl} = l + 1 \quad (7)$$

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

The correlation orbital exponents are given in table 2.

2.2. Transition probabilities

In evaluating the transition probabilities of intercombination lines it is necessary to include the J-dependent relativistic operators (spin-orbit, spin-other-orbit and spin-spin) in the Hamiltonian. Hence we have to use a J-dependent CI expansion which takes the form

$$\Psi(J, M_J) = \sum_j a_j \Phi_j(\alpha_j L_j S_j J M_J) \quad (8)$$

where $\{\Phi_j\}$ denotes a set of single-configuration wavefunctions, $\{\alpha_j\}$ defines the coupling of the angular momenta of the electrons,

$$J = L_j + S_j \quad (9)$$

for each j , and $\{a_j\}$ are determined as the components of the appropriate eigenvector of the Hamiltonian matrix with basis $\{\Phi_j\}$. In accordance with the previous section the Hamiltonian consists of the usual non-relativistic terms, the one-electron J-independent relativistic operators and the J-dependent relativistic operators.

The coefficients $\{a_j\}$ are evaluated using the computer code CIV3 (Hibbert 1975) modified (Glass and Hibbert 1979) to include these relativistic effects: each is expressed as a product of irreducible tensors whose matrix elements are calculated using Racah algebra techniques (Fano et al 1963).

In table 3 a list of configurations used in each state is given. The first four wavefunctions are LS coupled and are used in the expansion for the last two intermediate-coupled wavefunctions. Using these CI wavefunctions we evaluated the emission electric dipole transition probabilities.

3. Results and Discussions

Armstrong et al (1976) have calculated the intercombination transition probabilities $2s\ 2p\ ^3P_1^0 \rightarrow 2s^2\ ^1S_0$ for the beryllium sequence using the relativistic multiconfigurational Hartree-Fock method. In their calculation they represented the ground state wavefunction $\Psi(2s^2\ ^1S_0)$ by the configurations $2s^2\ ^1S_0$, $2p^2\ ^1S_0$, 3P_0 and the excited state wavefunction, $\Psi(2s\ 2p\ ^3P_1^0)$, by the configurations $2s\ 2p\ ^3P_1^0$, $^1P_1^0$. As a starting point we used the same CI expansion. The results are presented in table 4 calculation a: and b:. Calculation a: represents the results obtained by only including the one-electron relativistic operators as well as the usual non-relativistic terms in the Hamiltonian while in calculation b: the spin-other-orbit and spin-spin terms are also included.

For krypton and molybdenum calculation a: and b: are in very good agreement, however, for tungsten they differ by approximately 20%. It is seen that (i) the energy splitting $E(^1S_0 \rightarrow ^3P_1^0)$ between the two states in a transition is increased when the spin-other-orbit and spin-spin interactions are included in the Hamiltonian. For example, for molybdenum the energy of the $2s^2\ ^1S_0$ state is raised approximately 0.005 au while the energy of the upper state $2s\ 2p\ ^3P_1^0$ is raised 0.2 au when the spin-other-orbit and spin-spin terms are included. (ii) The fine-structure splittings, $E(^3P_1^0 - ^3P_0^0)$, $E(^3P_2^0 - ^3P_1^0)$ are reduced when the two-body J-dependent relativistic terms are included.

Comparing our results with those of Armstrong et al (1976) calculation e: of table 4 for krypton and molybdenum agreement is very good. For tungsten agreement is within 20% for the oscillator strength. Weis (1976) has calculated the $2s\ 2p\ ^3P_1^0 \rightarrow 2s^2\ ^1S_0$ transition probability for krypton and molybdenum. For krypton agreement is excellent, within 2% while for molybdenum agreement is within 10%.

The next stage of our investigation was to study the effect of including correlation functions in the wavefunctions. We repeated the calculations using the wavefunctions listed in table 3. The results are presented in table 4 calculation c: and d: (calculation c: represents the effect of including the one-electron relativistic operators in the Hamiltonian, d: spin-other-orbit and spin-spin interactions are also included).

It is seen that agreement between the "simpler" method (calculation c:) and calculation d: where the Breit-Pauli effects are included is excellent. In our earlier work on the beryllium sequence we found that for intercombination transitions Breit-Pauli effects were important. This is partly due to the fact that intercombination transition probabilities are highly sensitive to the values of the very small coefficients in the CI expansion of the wavefunction. For krypton, molybdenum and tungsten the coefficient of the $2s\ 2p\ ^1P_1^0$ configuration in the $^3P_1^0$ wavefunction ranges from 0.3 to 0.5 compared to, for example, neon where it is only 0.003. Also the contribution to the energy from the spin-other-orbit and spin-spin interactions goes as $\alpha^2 Z^3$ (α is the fine-structure constant), whereas the contribution from the one-electron relativistic operators goes as $\alpha^2 Z^4$.

Comparing the results obtained from the new calculation with those obtained using only configurations formed within the $n = 2$ complex, for krypton agreement is fairly good. However, agreement becomes progressively worse for molybdenum and tungsten. For example, for tungsten they differ by a factor of five.

In order to try and explain the discrepancies between the results we will consider molybdenum (similar argument applies to krypton and tungsten).

Including correlation functions in the wavefunctions changes the energies of the $2s^2 1S_0$ and $2s 2p^3 P_1^0$ states from -219.44862 au to -2194.17840 au and from -2188.16234 au to -2190.20510 au respectively. Thus the energy splitting $E(1S_0 \rightarrow 3P_1^0)$ between the two states is increased when correlation functions are included in the CI expansion. The important additional configuration in the $2s^2 1S_0$ wavefunction is $2s 3s$, mixing coefficient is 0.13. The importance is due to spin-orbit coupling with the $3P_0$ configurations, since its coefficient in an LS coupled $1S$ state is essentially zero.

Similarly we see that the fine-structure splitting $E(3P_1^0 - 3P_0^0)$ is decreased and $E(3P_2^0 - 3P_1^0)$ fine-structure splitting is increased when a more elaborate wavefunction is used. The main contribution to this effect comes from the $3P_1^0$ level. Inclusion of correlation functions in the CI expansion lowers the $3P_1^0$ energy more than that of $3P_0^0$ and $3P_2^0$. The importance is due to spin-orbit coupling of $2s 3p^1 P_1^0$ configuration with the $3P_1^0$ configurations.

The oscillator strength is also increased when correlation effects are included. In our previous work on the $2s 2p^3 P_1^0 \rightarrow 2s^2 1S_0$ intercombination line we found that the dominant contributions to the matrix elements come from the interaction involving HF configurations $\langle 2s^2 1S_0 | \sum_i \mathbf{r}_i | 2s 2p^1 P_1^0 \rangle$, $\langle 2p^2 3P_0 | \sum_i \mathbf{r}_i | 2s 2p^3 P_1^0 \rangle$ and $\langle 2p^2 1S_0 | \sum_i \mathbf{r}_i | 2s 2p^1 P_1^0 \rangle$. For krypton, molybdenum and tungsten the next most important term after $\langle 2s^2 1S_0 | \sum_i \mathbf{r}_i | 2s 2p^1 P_1^0 \rangle$ was not $\langle 2p^2 3P_0 | \sum_i \mathbf{r}_i | 2s 2p^3 P_1^0 \rangle$ as we had expected, but rather $\langle 2p^2 1S_0 | \sum_i \mathbf{r}_i | 2s 2p^1 P_1^0 \rangle$. As in our earlier work we found that the next most important contribution was $\langle 2s^2 1S_0 | \sum_i \mathbf{r}_i | 2s 3p^1 P_1^0 \rangle$ and not $\langle 2p^2 1S_0 | \sum_i \mathbf{r}_i | 2p 3d^1 P_1^0 \rangle$. For krypton,

molybdenum and tungsten the contribution from the matrix element $\langle 2p^2 1S_0 | \sum_i r_i | 2p 3d 1P_1^0 \rangle$ is almost negligible. In contrast to the lower members of the sequence there are also important contributions from matrix elements $\langle 2s 3s 1S_0 | \sum_i r_i | 2s 2p 1P_1^0 \rangle$, $\langle 2s 3s 1S_0 | \sum_i r_i | 3s 2p 1P_1^0 \rangle$, $\langle 2s 3s 1S_0 | \sum_i r_i | 2s 3p 1P_1^0 \rangle$ and $\langle 2p 3p 3P | \sum_i r_i | 2s 2p 3P_1^0 \rangle$. In table 5 we list mixing coefficients of the important configurations and in table 6 corresponding contributions to the matrix elements are listed.

Agreement with other theoretical calculations is now disappointing. This is in contrast to the allowed transition $2s^2 1S_0 \rightarrow 2s 2p 1P_1^0$ where agreement between our theoretical calculations including correlation functions in the CI expansion and those of Armstrong et al (1976) where correlation effects were omitted, Weiss (1976), Lin and Johnson (1977) for krypton and molybdenum were very good. However, it is worth noting that in their (Armstrong et al, Weiss Lin and Johnson) calculations they used the same radial functions for both transitions, whereas we have used a different set of radial functions for each calculation.

To investigate if this was the cause for the large discrepancy between our results and other theoretical calculations we repeated the calculations using the wavefunctions from our previous work (Glass 1979b) for allowed transitions. The $1s$, $2s$, $2p$ HF functions are now those of the $2s 2p 1P^0$ state and the correlation functions $3s$, $3p$, $3d$, $4f$ are those optimized on the $2p^2 1D$ state. In table 7, for completeness, a list of configurations used in each state formed from the new functions are given. We present the results of the new calculation in table 8.

It is seen that the results obtained using the CI expansion including only configurations which can be formed within the $n = 2$ complex,

calculation a: and b:, are in excellent agreement with those of Armstrong et al (1976), calculation e:, and Weiss (1976), calculation f: However, when correlation effects are included the results are again drastically changed especially for tungsten. Comparing the calculations obtained by both methods, table 4 and 8 we see that the energy splitting $E(^1S_0 \rightarrow ^3P_1^0)$, oscillator strength, transition probabilities and fine-structure splitting of the $2s\ 2p\ ^3P_J^0$, $J = 0, 1, 2$ levels for krypton and molybdenum are independent of whether we use the $1s, 2s, 2p$ HF functions determined on the $2s\ 2p\ ^3P^0$ or $^1P^0$ state, calculation a: and b:. For tungsten with the exception of the fine-structure splitting agreement is not as good. However, when we include correlation functions in the CI expansion agreement between the two calculations is disappointing. To investigate further the discrepancies in the two methods we also list in table 5 mixing coefficients of the important configurations for molybdenum from method II and in table 6 corresponding contributions to the matrix elements are listed.

From table 5 it is seen that the coefficients of configurations formed from HF functions, with exception of $2p^2\ ^1S_0$, 3P_0 configurations, are independent of those of HF and correlation functions. Whereas, for example, the coefficient of $2p^2\ ^3P_0$ configuration changes by 16% depending on how the correlation functions are determined. This change is due to (i) interaction between $2p^2$ and $2p\ 3p$ configurations and (ii) spin-orbit coupling of $2p^2\ ^3P_0$ with $2s\ 3s\ ^1S_0$ configuration. Furthermore, from table 6 we see that the dominant contribution, $\langle 2s^2\ ^1S_0 | \sum_i \mathbf{L}_i | 2s\ 2p\ ^1P_1^0 \rangle$, is independent of those of HF functions. Also from table 6 it is seen that cancellation effects are greater when the second method is used. However, it is interesting that using either method the important additional configuration to those formed from within the $n = 2$ complex is $2s\ 3p\ ^1P^0$.

The importance of this configuration has been discussed in detail in an earlier publication (Glass and Hibbert 1978).

In this paper we have presented some fairly extensive CI calculations of energy splittings, wavelengths, oscillator strengths, transition probabilities and fine-structure splittings for krypton, molybdenum and tungsten. We see that good agreement with other theoretical calculations can be obtained if we only include in the CI expansion all configurations which can be formed from the $n = 2$ complex. Also if we use the same wavefunctions for both allowed and intercombination transitions agreement, in particular for tungsten, with the theoretical calculation of Armstrong et al is improved. Furthermore, including correlation effects in the wavefunction changes the results drastically. This is due to the contribution from the matrix element $\langle 2s^2 1S_0 | \sum_i \mathbf{r}_i | 2s 3p 1P_1^0 \rangle$. As in our previous work we see that (table 6) the cause of the large effect of the $2s 3p 1P_1^0$ configuration, is independent of how the HF functions are determined. The importance is due to spin-orbit coupling with the $3P_1^0$ configurations, since its coefficient in an LS coupled $1P^0$ state is essentially zero. Thus in calculating intercombination transition probabilities ($2s 2p 3P_1^0 \rightarrow 2s^2 1S_0$) the $2s 3p 1P^0$ configuration should be included.

The major unresolved question is that of how the relativistic effects should be included and of what changes they induce in the wavefunction. Armstrong et al (1976) in determining relativistic radial wave functions included in the calculation of the wavefunction interactions which in the Pauli approximation becomes the nuclear spin-orbit and part of the spin-other-orbit interactions. In the calculations reported in this paper the radial functions used in the final calculations were determined in an LS

coupled representation of the atomic states. The nuclear spin-orbit, spin-other-orbit, spin-spin, Darwin and mass-correction contributions were then included in the Hamiltonian in order to determine the configuration mixing. Our results, calculation c: table 4 and 8 are in excellent agreement with those of Armstrong et al calculation e: table 4 and 8.

For the same reasons, the way the correlation functions are to be chosen is not as clear as for allowed transitions. One would prefer to use the relativistically coupled $J = 1$ energy. But this is dominated by the $^3P_1^0$ configurations, whereas the transition probability whose value we wish to determine depends more crucially on the relative weight of the $^1P_1^0$ configurations. In our previous work the np ($n \geq 3$) functions were determined on the non-relativistic $^1P^0$ energy which, because it reproduces reasonably well the fine-structure splitting, is satisfactory for determining wavefunctions for use in the calculation of atomic properties involving fine-structure levels. Unfortunately, at present, there are no experimental fine-structure splittings for krypton, molybdenum and tungsten for us to compare our results with.

In calculating the transition energies, fine-structure splittings and transition probabilities for intercombination line $2s\ 2p\ ^3P_1^0 \rightarrow 2s^2\ ^1S_0$ it is worth noting that we have only included the relativistic corrections. However, for highly ionized atoms quantum electrodynamics effects, for example, the Lamb Shift should perhaps also be included. Thus these highly ionized atoms are a sensitive test of the theoretical treatment of relativistic effects and quantum electrodynamics effects.

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Table 1: Hartree-Fock function parameters.

$n\ell$	$I_{jn\ell}$	Kr XXXIII	Mo XXXIX	W LXXI
		$\zeta_{jn\ell}$		
1s	1	35.48208	41.48266	73.08288
1s	1	58.56722	68.22717	108.15586
2s	2	16.86457	19.83462	35.71899
2s	2	20.65474	25.03535	45.74280
2s	2	28.75102	33.8705	60.53205
2p	2	16.55619	19.51604	35.47729
2p	2	17.95682	21.00843	37.02513
2p	2	17.69306	20.65415	36.24642
2p	2	39.62143	46.31449	79.00994
		$C_{jn\ell}$		
1s		-0.98558	-0.98738	0.98937
		-0.01228	-0.01068	0.01357
		0.00011	0.00012	-0.00075
		0.00034	0.00027	0.00264
		-0.00456	-0.00403	-0.00448
2s		0.34576	0.34828	-0.36048
		-0.00168	-0.00211	0.00528
		-1.43483	-1.43453	1.46670
		0.15645	0.16610	-0.20643
		0.28819	0.27811	-0.26536
2p		0.71062	0.69823	0.76787
		0.23767	0.24882	0.36084
		0.04875	0.05033	-0.13078
		0.00580	0.00505	0.00341

Table 2: Correlation orbital exponents.

$n\ell$	I_{jnl}	ζ_{jnl}		
		Kr XXXIII	Mo XXXIX	W LXXI
3s	1	17.67431	20.57398	35.26963
	2	18.01801	21.21421	35.12363
	3	17.99008	21.11708	37.67061
3p	2	13.59781	15.97692	28.55855
	3	17.50585	20.57913	36.89268
3d	3	19.05854	22.42091	40.35787
4p	2	14.72604	17.34998	31.77609
	3	14.73216	17.34992	31.63490
	4	16.69891	19.66470	35.68611
5p	2	24.8319	29.23755	51.13674
	3	24.8319	29.23755	51.13674
	4	24.8319	29.23755	51.13674
	5	24.8319	29.23755	51.13674

Table 3: Configurations used for each state.

State	Configurations
$\Psi(2s^2 1s)$	$[1s^2] 2s^2, 2s 3s, 3s^2, 2p^2, 2p 3p, 3p^2, 3d^2$
$\Psi(2s 2p^3 P_0^0)$	$[1s^2] 2s 2p, 2s 3p, 3s 2p, 3s 3p, 2p 3d, 3p 3d$
$\Psi(2s 2p^1 P_0^0)$	$[1s^2] 2s 2p, 2s 3p, 3s 2p, 3s 3p, 2p 3d, 3p 3d, 2s 4p, 3s 4p, 2s 5p, 3s 5p$
$\Psi(2p^2 3P)$	$[1s^2] 2p^2, 2p 3p, 3p^2, 3d^2$
$\Psi(2s^2 1s_0)$	$\Psi(2s^2 1s_0), \Psi(2p^2 3P_0)$
$\Psi(2s 2p^3 P_1^0)$	$\Psi(2s 2p^3 P_1^0), \Psi(2s 2p^1 P_1^0)$

Table 4: Energy differences, wavelength $\{\lambda\}$, oscillator strength $\{f_l\}$ and transition probabilities $\{A\}$ for the intercombination transition $2s^2 1S_0 \rightarrow 2s 2p^3 P_1^0$

	Unit	Calculation	Kr XXXIII	Mo XXXIX	W LXXI
$E(1S_0 \rightarrow 3P_1^0)$	au	a	2.5796	3.1273	6.2378
		b	2.6721	3.2863	7.2102
		c	2.8179	3.7795	40.2777
		d	2.9249	3.9733	42.4113
		e	2.754	3.427	8.491
$\lambda(1S_0 \rightarrow 3P_1^0)$	Å	a	176.6	145.7	73.0
		b	170.5	138.6	60.3
		c	161.7	120.6	11.3
		d	155.8	114.7	10.7
		f	173.0	141.6	
$f_l(1S_0 \rightarrow 3P_1^0)$		a	0.545(-2) [†]	0.739(-2)	0.889(-2)
		b	0.535(-2)	0.762(-2)	0.108(-1)
		c	0.631(-2)	0.947(-2)	0.510(-1)
		d	0.624(-2)	0.980(-2)	0.543(-1)
		e	0.54(-2)	0.75(-2)	0.99(-2)
		g		0.589(-2)	
$A(3P_1^0 \rightarrow 1S_0)$	$\times 10^8 \text{Sec}^{-1}$	a	3.88	7.74	37.05
		b	4.09	8.81	60.26
		c	5.36	14.49	8866.48
		d	5.72	16.57	10456.1
		f	4.02	8.16	
$E(3P_1^0 - 3P_0^0)$	cm^{-1}	a	89190	125583	294914
		b	83186	118060	264658
		c	86464	111043	3655552*
		d	80194	102780	3675168
$E(3P_2^0 - 3P_1^0)$	cm^{-1}	a	437228	871829	9880903
		b	403595	815055	9539926
		c	485629	1009805	19213089
		d	448253	944340	18594548

[†]The notation implies $\alpha \times 10^\beta$

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- c: CI (Non-relativistic + one-electron mass correction + one-electron Darwin term + nuclear spin-orbit interaction)
- d: CI (Non-relativistic + one-electron mass correction + one-electron Darwin term + nuclear spin-orbit + spin-other-orbit + spin-spin interactions)

Table 4 Continued

e: Armstrong et al (1976)

f: Weiss (1976)

g: Lin and Johnson (1977)

* including only the configurations which can be formed within the $n = 2$ complex

Table 5: Mixing coefficients of the important configurations
for the intercombination transition $2s^2 1S_0 \rightarrow 2s 2p^3 1P_1^0$
in Mo XXXIX

Configurations	Wavefunction listed in table 3	Wavefunction listed in table 7
$2s^2 1S_0$	0.9812	0.9809
$2p^2 1S_0$	-0.1374	-0.1461
$2s 3s 1S_0$	0.1256	-0.1139
$2p^2 3P_0$	-0.0502	-0.0579
$2p 3p 3P_0$	-0.0057	-0.0068
$2s 2p^3 1P_1^0$	0.9041	0.9082
$2s 2p^3 1P_1^0$	0.4147	0.4073
$2s 3p^3 1P_1^0$	0.0252	0.0291
$3s 2p^3 1P_1^0$	0.0358	-0.0311
$2p 3d^3 1P_1^0$	0.0067	-0.0065

Table 6: The more important contributions to the matrix elements
for the intercombination transitions $2s^2 1S_0 \rightarrow 2s 2p^3 3P_1^0$
in Mo XXXIX

Configurations	Wavefunction listed in table 3	Wavefunction listed in table 7
$2s^2 1S_0 \rightarrow 2s 2p^3 1P_1^0$	-0.1296	0.1272
$2p^2 1S_0 \rightarrow 2s 2p^3 1P_1^0$	0.0105	-0.0109
$2p^2 3P_0 \rightarrow 2s 2p^3 3P_1^0$	0.0083	-0.0097
$2s^2 1S_0 \rightarrow 2s 3p^3 1P_1^0$	0.0052	-0.0065
$2s 3s 1S_0 \rightarrow 2s 2p^3 1P_1^0$	0.0028	-0.0025
$\quad \quad \quad \rightarrow 3s 2p^3 1P_1^0$	-0.0010	0.0008
$\quad \quad \quad \rightarrow 2s 3p^3 1P_1^0$	-0.0006	0.0008
$2p 3p^3 3P_0 \rightarrow 2s 2p^3 3P_1^0$	-0.0005	0.0006
$2p^2 1S_0 \rightarrow 2p 3d^3 1P_1^0$	-0.0003	0.0003

Table 7: List of configurations used for each state

State	Configurations
$\Psi(2s^2 1S)$	$[1s^2] 2s^2, 2p^2, 2s 3s, 3s^2, 2p 3p, 3p^2, 3d^2$
$\Psi(2p^2 3P)$	$[1s^2] 2p^2, 2p 3p, 3p^2, 3d^2$
$\Psi(2s 2p 3P^0)$	$[1s^2] 2s 2p, 2s 3p, 3s 2p, 3s 3p, 2p 3d, 3p 3d, 3d 4f$
$\Psi(2s 2p 1P^0)$	$[1s^2] 2s 2p, 2s 3p, 3s 2p, 3s 3p, 2p 3d, 3p 3d, 3d 4f$
$\Psi(2s^2 1S_0)$	$\Psi(2s^2 1S_0), \Psi(2p^2 3P_0)$
$\Psi(2s 2p 3P_1^0)$	$\Psi(2s 2p 3P_1^0), \Psi(2s 2p 1P_1^0)$

Table 8: Energy differences, wavelength $\{\lambda\}$, oscillator strength $\{f_\ell\}$ and transition probabilities $\{A\}$ for the intercombination transition $2s^2 1S_0 \rightarrow 2s 2p^3 3P_1^0$

	Unit	Calculation	Kr XXXIII	Mo XXXIX	W LXXI
$E(1S_0 \rightarrow 3P_1^0)$	au	a	2.5208	3.0372	5.7268
		b	2.6143	3.1974	6.6977
		c	2.7026	3.4056	15.1905
		d	2.8083	3.5958	16.9073
		e	2.754	3.427	8.491
$\lambda(1S_0 \rightarrow 3P_1^0)$	Å	a	180.8	150.0	79.6
		b	174.3	142.5	47.3
		c	168.6	133.8	30.0
		d	162.2	126.7	26.9
		f	173.0	141.6	
$f_\ell(1S_0 \rightarrow 3P_1^0)$		a	0.540(-2) [†]	0.719(-2)	0.792(-2)
		b	0.531(-2)	0.745(-2)	0.985(-2)
		c	0.568(-2)	0.775(-2)	0.168(-1)
		d	0.562(-2)	0.807(-2)	0.191(-1)
		e	0.54(-2)	0.75(-2)	0.99(-2)
		g		0.589(-2)	
$A(3P_1^0 \rightarrow 1S_0)$	$\times 10^8 \text{Sec}^{-1}$	a	3.68	7.11	27.82
		b	3.89	8.15	47.31
		c	4.44	9.63	416.03
		d	4.74	11.17	584.57
		f	4.02	8.16	
$E(3P_1^0 - 3P_0^0)$	cm^{-1}	a	89202	125317	293891
		b	83254	117858	263726
		c	91552	129470	315462
		d	85521	121751	270320
$E(3P_2^0 - 3P_1^0)$	cm^{-1}	a	442759	881047	9934604
		b	408762	823782	9592121
		c	478044	986721	14721246
		d	440942	921881	14197548

[†] The notation implies $\alpha \times 10^\beta$

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- c: CI (Non-relativistic + one-electron mass correction + one-electron Darwin term + nuclear spin-orbit interaction)
- d: CI (Non-relativistic + one-electron mass correction + one-electron Darwin term + nuclear spin-orbit + spin-other-orbit + spin-spin interactions)

Table 8 Continued

e: Armstrong et al (1976)

f: Weiss (1976)

g: Lin and Johnson (1977)

* including only the configurations which can be formed within the $n = 2$ complex

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