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Semi-empirical calculations of radiative decay rates in Mo II. A comparison between oscillator strength parametrization and core-polarization-corrected relativistic Hartree-Fock approaches

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ABSTRACT

We present a semi-empirical determination of Mo II radiative parameters in a wide wavelength range 1716–8789 Å. Our fitting procedure to experimental oscillator strengths available in the literature permits us to provide reliable values for a large number of Mo II lines, predicting previously unmeasured oscillator strengths of lines involving $4d^45p$ and $4d^35s5p$ odd-parity configurations. The extracted transition radial integral values are compared with ab-initio calculations: on average they are 0.88 times the values obtained with the basic pseudo-relativistic Hartree Fock method and they agree well when core polarization effects are included. When making a survey of our present and previous studies and including also those given in the literature we observe as general trends a decreasing of transition radial integral values with filling nd shells of the same principal quantum numbers for $nd^k(n+1)s \rightarrow nd^k(n+1)p$ transitions.

1. Introduction

Molybdenum is an element of the 4d-shell transition group. There are 33 known isotopes of molybdenum (Mo) ranging in atomic mass from 83 to 115, as well as 4 metastable nuclear isomers. Seven isotopes occur naturally, with atomic masses of 92, 94, 95, 96, 97, 98, and 100. Historically, it is in 1926 that Meggers and Kiess initiated the level structure analysis of singly ionized molybdenum, establishing 27 levels [1]. Later on, Schauls and Sawyer [2] extended this first study. It is in 1958 that a big extension of this study occurred, performed by Kiess alone this time, giving furthermore 179 experimental Landé-factor values of levels [3]. This good compilation had constituted in its day a masterpiece of clarity and accuracy and showed the presence of strong intuition. More recently, after a break of a half century nearly a full fine structure (fs) study was published [4]: the spectrum of Mo II has been recorded with Fourier transform spectrometers in the wavelength interval 1500–7000 Å and 110 new levels were reported. Furthermore an accurate theoretical analysis of 5 even-parity configurations and 2 odd-parity configurations was performed. In our recent analysis devoted mainly to Mo II hyperfine structure (hfs) we have dealt beforehand with fine structure level study [5] to obtain level eigenvectors, in order to work in intermediate coupling; we confirm the validity of the excellent huge work of H. Nilsson and J. C. Pickering [4], since when we have recurred to the extracted level eigenvectors from this work in order to compute hfs data, the latter give a satisfactory agreement with new and accurate experimental hfs data of Rosner and Holt [6]. We have only to point out that the two levels of $(^3D)5p\ w^2D$, at 72,039.362 cm^{-1} and 72,829.914 cm^{-1} should have their total angular momentum J designations inverted [3,5]. In an extension of these Mo II electronic structure studies previously cited, relative experimental oscillator strengths of 58 Mo II lines were determined by Schnehage et al. [7] but their investigations covered only the region 2700–5700 Å; this limitation did not permit them to reach ranging in wavelength transitions involving the ground term levels. Historically, in the same year Hannaford and Lowe [8] measured lifetimes of 15 Mo II levels. Eighteen years later Sikström et al. [9] reported experimental branching fraction values, ranging in the wavelength from 1970 to 4370 Å and radiative lifetime measurements for 10 levels. We have to mention also the complementary extensions on the same subject, done by Lundberg et al. [10] and Jiang et al. [11]. Recently a Spanish team has presented numerous new oscillator strength measurements, arising mainly from highly excited levels [12,13]. Laser-induced plasma generated from a fused glass sample was used to obtain radiative parameters via laser-induced breakdown spectroscopy. Theoretically, in [14] Quinet had calculated ra-

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diative lifetimes and oscillator strengths within the framework of the pseudo-relativistic Hartree Fock (HFR) method, including core polarisation effects. Nilsson and Pickering [4] present HFR oscillator strengths for all their classified lines. In turn in this study we propose to perform Mo II oscillator strength data recurring to semi-empirical oscillator strength parametrization (OSP) method and to compare our data with those given previously in the literature and to predict those which are missing with help of the pseudo-relativistic Hartree Fock (HFR) method, including core polarisation effects.

2. Oscillator strength calculation

We open this paragraph by evoking the inescapable relations we have made use in this work: the oscillator strength $f(\gamma\gamma')$ for the transition between two levels $|\gamma J>$ and $|\gamma' J'>$ of an atom or molecule with statistical weights $g=(2J+1)$ and $g'=(2J'+1)$ respectively, is a dimensionless physical quantity, expressing the probability of absorption or emission in this transition between these two levels and related to the transition probability $W(\gamma\gamma')$ by [15]:

$$W(\gamma\gamma') = \frac{2\omega^2 e^2}{mc^3}\left|f(\gamma\gamma'\right| \tag{1}$$

where m and e are the electron mass and charge, c is the velocity of light, γ describes the initial quantum state, $\omega=[E(\gamma)-E(\gamma')]/\hbar$, $E(\gamma)$ is the energy of the initial state. The quantities with primes refer to the final state.

For the electric dipole transitions, the weighted oscillator strength gf is related to the line strength $\boldsymbol{S}$ [15]:

$$gf = 8\pi^2 mca_0^2\frac{\sigma}{3h}S = 303.76\times10^{-8}\sigma\ S \tag{2}$$

where a_0 is the Bohr radius, $\sigma=|E(\gamma)-E(\gamma')|\ /\ hc$ and h is the Planck's constant.

The electric dipole line strength is defined by:

$$S = \left|\left\langle \gamma J\middle\| P^1\middle\|\gamma' J'\right\rangle\right|^2 \tag{3}$$

The tensorial operator $\boldsymbol{P^1}$ (in units of ea_0) in the reduced matrix element stands for the electric dipole moment.

To obtain the gf value, we need to calculate initially $\boldsymbol{S}$, or preferably its square root. For multiconfiguration system, the wavefunctions $|\gamma J>$ and $|\gamma' J'>$ are expanded in terms of a set of basis functions $|\phi\ S\ L\ J>$ and $|\phi'\ S'L'J'>$, respectively:

$$|\gamma J\rangle = \sum_i c_i|\phi SLJ\rangle \quad \text{and} \quad \left|\gamma' J'\right\rangle = \sum_j c_j{}'\left|\phi' S'L'J'\right\rangle \tag{4}$$

The square root of the line strength may be written in the following form:

$$S^{1/2}_{\gamma\gamma'} = \sum_i\sum_j c_i c_j{}'\left\langle\phi SLJ\middle\| P^1\middle\|\phi' S'L'J'\right\rangle \tag{5}$$

The appropriate computer program [16] calculates the angular part of the matrix element $<\phi\ S\ L\ J\ ||P^1||\phi' S'L'J'>$. From Eqs. (2) and (5), we can express the gf-values as a linear combination:

$$(gf)^{1/2} = \sum_{nl,n'l'}(303.76\times10^{-8}\sigma)^{1/2} \times\sum_i\sum_j c_i c_j{}'\left\langle\phi SLJ\middle\| P^1\middle\|\phi' S'L'J'\right\rangle \tag{6}$$

where σ is the wavenumber, given in cm $^{-1}$, and the sum extends over all possible transitions ($ns\leftrightarrow n$'p, $nd\leftrightarrow n$'p, $nd\leftrightarrow n$'f).

The weighted transition probability is [15]:

$$gA = (2J'+1)A = \frac{64\pi^4 e^2 a_0}{3h}\sigma^3 S = 2.0261\times10^{-6}\sigma^3 S \tag{7}$$

Table 1
Mo II Transition radial integral values.

Transition	HFR[a]	HFR+CPOL[b]	OSP[c]
$4d^45s$–$4d^35s5p$	1.8848	1.5224	
$4d^45s$–$4d^45p$	3.4247	2.9597	2.8558 (0.0084)
$4d^5$–$4d^45p$	2.0962	1.7665	1.725 (0.010)
$4d^35s^2$–$4d^35s5p$	3.2856	2.7753	

[a] Relativistic Hartree Fock method
[b] Relativistic Hartree Fock method including core-polarization
[c] Oscillator strength parametrization method

where σ is given, as previously, in cm^{-1} and S in atomic units of $e^2a_0^2$. Substitution of Eq. (1) into (7) leads to:

$$(2J'+1)A = 0.66702\ \sigma^2 gf \tag{8}$$

In the present study, our aim is to evaluate at first line strengths using Eq. (5). As in previous work devoted to oscillator strength determination (see for instance [16]), the angular coefficients of the transition matrix, obtained in pure SL coupling with help of Racah algebra is transformed into the actual intermediate coupling recurring to our level eigenvector amplitudes previously derived. Moreover the transition integrals

$$\int_0^\infty P_{nl}(r)\ r\ P_{n'l'}(r)\ dr \tag{9}$$

are treated as free parameters in the least squares fit to experimental gf values. Up to now only $4d^5$–$4d^45p$ and $4d^45s$–$4d^45p$ Mo II transition oscillator strengths have been measured. We have initially selected the strongest lines, not blended, whose experimental gf values were published very recently [12,13], with the best accuracy and particularly those representing transitions between levels with a limited number of leading components as shown in [4]; then, for these $4d^45s$–$4d^45p$ and $4d^5$–$4d^45p$ transitions we have extracted semi-empirically, with very good accuracy, the radial integral values, reported in Table 1. In the same table, we also give the results computed by means of the pseudo-relativistic Hartree Fock (HFR) method using the basic Cowan code [17] and including core-polarization (HFR+CPOL), as described in [18,19]. As a reminder, in the latter approach, the radial dipole integrals given in Eq. (9) are replaced by

$$\int_0^\infty P_{nl}(r)\ r\left[1-\frac{\alpha_d}{(r^2+r_c^2)^{3/2}}\right]P_{n'l'}(r)\ dr - \frac{\alpha_d}{r_c^3}\int_0^{r_c} P_{nl}(r)\ r\ P_{n'l'}(r)\ dr \tag{10}$$

where a_d is the dipole polarizability of the ionic core, for which numerical values can be found in the literature (see e.g. [20]), and r_c is the cut-off radius that is arbitrarily chosen as a measure of the size of the ionic core. In practice, this parameter is usually chosen to be equal to the HFR mean value $<r>$ for the outermost ionic core orbital.

When looking at Table 1, one can observe that *ab initio* HFR radial dipole integrals are about 20% larger than the values extracted from our oscillator strength parametrization (OSP) approach while the difference is reduced to a few percent when considering the HFR+CPOL results obtained using a Mo IV ionic core, as reported in [10,11]. In the same Table, for further analysis, we have also added HFR and HFR+CPOL radial integral values for transitions involving the $4d^35s5p$ configuration.

In Table 2, we have gathered the radial integral values of $nd^k(n+1)s$ –> $nd^k(n+1)p$ transitions, obtained semi-empirically in our previous works, using the same code, for singly ionized atoms, such as V II [21], Zr II [22], Nb II [23], Rh II [24], Hf II [25] to which we have added those given by Ruczkowski et al. for Sc II [16] and Ti II [26]. It is easy to observe that these transition radial

Table 2
ns → np transition radial integral values of some singly ionized atoms.

ion	Z	Transition	HFR[a]	HFR+CPOL(III)[b]	HFR+CPOL(IV)[c]	OSP[d]	OSP/HFR
Sc II	20	3d4s 3d4p	3.6199	3.2827	3.4201	3.413 (0.018) [26]	0.94
Ti II	22	$3d^2$4s $3d^2$4p	3.4511	3.0921	3.2530	3.078 (0.015) [21]	0.89
V II	23	$3d^3$4s $3d^3$4p	3.3085	2.9334	3.1035	3.0346 (0.0094) [27]	0.92
Zr II	40	$4d^2$5s $4d^2$5p	3.7111	2.9731	3.3361	3.15 (0.02) [22]	0.85
Nb II	41	$4d^3$5s $4d^3$5p	3.5556	2.7842	3.1144	3.0605 (0.0059) [23]	0.86
Mo II	42	$4d^4$5s $4d^4$5p	3.4247	2.6478	2.9597	2.8558 (0.0084)	0.83
Rh II	45	$4d^7$5s $4d^7$5p	3.1238	2.3680	2.6374	2.7426 (0.0007) [24]	0.88
Hf II	72	$5d^2$6s $5d^2$6p	3.4833	2.6500	3.0284	2.984* (0.013) [25]	0.86

[a] Relativistic Hartree Fock method.
[b] Relativistic Hartree Fock method including core-polarization with a 2+ ionic core.
[c] Relativistic Hartree Fock method including core-polarization with a 3+ ionic core.
[d] Oscillator strength parametrization method.
* There is a typo in paper [25] from where we have taken this value.

integral values decrease with the filling of *n*d-shells for the same principal quantum number; this behaviour is different for instance from established general trends in the hyperfine structure analyses: increasing (contrary to the transition radial integral which is rather decreasing) of the most influential s-monoelectronic hfs parameter divided by $g_I = \mu_I / I$, a_{ns}^{10}/g_I versus atomic number Z [27]. These remarks may serve, with resorting to any calculations, as hints at the starting of oscillator strength fitting procedure since we can use the deduced interval of our new investigated transition radial integral values with the help of those known for other ions and then we can conclude if our obtained data in the first stage are encouraging or not to carry on with our fitting procedure. For instance we propose intuitively $<nd^k(n+1)s|r^1|nd^k(n+1)p> = 3.00$ (0.02), 2.82 (0.02) and 2.78(0.02) respectively for $3d^44s$–$3d^44p$ in Cr II, $4d^55s$–$4d^55p$ in Tc II and $4d^65s$–$4d^65p$ in Ru II when having recourse to Table 2 (the value between parentheses shows the uncertainty).

In the latter table, we also give the radial dipole integrals calculated using the pseudo-relativistic Hartree Fock method without and with core-polarization corrections. It is interesting to note that the values deduced from our oscillator strength parametrization approach are on average 12% smaller than *ab initio* HFR results. It is also worthwhile to underline that the OSP data are generally very close to the HFR+CPOL values provided that an ionic core of the type of triply ionized species (IV) is considered in the latter approach. This can be rather easily explained by the fact that core-polarization effects are partially included in OSP calculations when considering configurations of the type $nd^{k-1}(n+1)s^2$ and $nd^{k-1}(n+1)s(n+1)p$, which correspond, for singly charged atoms, to a 3+ ionic core surrounded by 2 electrons.

3. Radiative data

The oscillator strengths obtained in our work with the semi-empirical oscillator strength parametrization (OSP) method are compared with the available experimental values [9,12,13] in Table 3 for Mo II spectral lines in the region 2000–4000 Å They are also compared with the values calculated using the HFR+CPOL approach. As the physical model considered in the latter method was exactly the same as the one described in our recent study of singly ionized molybdenum [10,11], the details will not be repeated here. Let us just remind that, in these works, the configurations $4d^5$, $4d^45s$, $4d^46s$, $4d^45d$, $4d^35s^2$, $4d^35p^2$, $4d^35d^2$, $4d^35s5d$ (even parity) and $4d^45p$, $4d^46p$, $4d^44f$, $4d^45f$, $4d^35s5p$, $4d^35p5d$ (odd parity) were included in the calculations with the dipole polarizability $\alpha_d = 5.67\ a_0{}^3$ [20] and the cut off radius $r_c = 1.73\ a_0$ as core-polarization parameters. This model was then combined with a semi-empirical adjustment of the radial parameters using the experimental energy levels published by Nilsson and Pickering [4], allowing us to optimize the average energies, the electrostatic interaction integrals and the spin-orbit parameters of $4d^5$, $4d^45s$, $4d^46s$,

Table 3
Comparison between calculated and experimental oscillator strengths in Mo II.

λ (Å)[a]	Lower level[b]		Upper level[b]		log gf			
	E (cm^{-1})	J	E (cm^{-1})	J	EXP[c]	$\Delta gf_{(exp)}$	OSP[d]	HFR+CPOL[d]
2079.985	15,331	7/2	63,393	5/2	−0.78	0.034	−0.91	−0.85
2080.473	15,447	11/2	63,498	9/2	−0.26	0.017	−0.16	−0.45
2081.680	0	5/2	48,023	3/2	−0.86	0.059	−0.85	−1.15
2111.248	15,691	5/2	63,042	5/2	−1.04	0.045	−0.95	−2.06
2113.819	15,199	5/2	62,492	7/2	−1.15	0.011	−1.23	−1.75
2119.710	15,331	7/2	62,492	7/2	−0.76	0.043	−0.89	−0.94
2122.698	15,331	7/2	62,426	5/2	−1.07	0.120	−1.00	−1.74
2170.614	15,691	5/2	61,747	3/2	−1.65	0.024	−1.57	−1.75
2187.622	17,344	5/2	63,042	5/2	−1.07	0.012	−1.21	−1.57
2341.592	15,199	5/2	57,892	7/2	−0.61	0.110	−0.81	−0.58
2467.337	22,980	11/2	63,498	9/2	−0.66	0.150	−0.84	−1.00
2515.080	22,980	11/2	62,729	11/2	−0.45	0.005	−0.52	−0.86
2538.457	13,461	9/2	52,843	9/2	−0.38	0.19	−0.31	−0.37
2542.672	12,901	7/2	52,218	7/2	−0.58	0.082	−0.79	−0.84
2551.021	23,854	7/2	63,042	5/2	−1.81	0.012	−2.00	−1.99
2588.779	23,935	5/2	62,551	3/2	−0.86	0.028	−0.89	−0.59
2596.420	24,509	7/2	63,013	9/2	−1.36	0.004	−1.57	−1.51
2602.800	11,784	1/2	50,192	3/2	−0.60	0.170	−0.58	−0.69
2618.465	24,372	1/2	62,551	3/2	−1.14	0.105	−1.10	−3.30

(*continued on next page*)

Table 3 (*continued*)

λ (Å)[a]	Lower level[b]		Upper level[b]		log gf			
	E (cm^{-1})	J	E (cm^{-1})	J	EXP[c]	$\Delta gf_{(exp)}$	OSP[d]	HFR+CPOL[d]
2619.344	11,784	1/2	49,950	1/2	−1.03	0.083	−0.96	−1.08
2620.050	25,342	7/2	63,498	9/2	−0.88	0.010	−1.00	−1.03
2638.761	12,418	5/2	50,303	7/2	−0.06	0.050	0.03	−0.07
2646.486	12,418	5/2	50,192	3/2	−0.29	0.260	−0.27	−0.38
2653.796	25,342	7/2	63,013	9/2	−0.76	0.010	−0.67	−0.87
2672.843	12,901	7/2	50,303	7/2	0.05	0.029	0.06	−0.06
2673.270	15,447	11/2	52,843	9/2	−0.12	0.054	−0.21	−0.29
2683.232	11,784	1/2	49,041	3/2	−0.23	0.045	−0.22	−0.28
2701.415	12,034	3/2	49,041	3/2	−0.34	0.058	−0.30	−0.33
2701.868	26,041	7/2	63,042	5/2	−0.41	0.010	−0.39	−0.30
2717.347	15,428	9/2	52,218	7/2	−0.41	0.009	−0.30	−0.37
2729.683	12,418	5/2	49,041	3/2	−0.92	0.024	−1.03	−0.95
2730.931	26,406	7/2	63,013	9/2	−1.06	0.023	−1.09	−0.90
2732.880	12,901	7/2	49,481	7/2	−0.47	0.027	−0.56	−0.56
2747.619	26,041	7/2	62,426	5/2	−0.41	0.029	−0.39	−1.29
2763.616	15,199	5/2	51,373	3/2	−0.56	0.039	−0.55	−0.61
2775.402	13,461	9/2	49,481	7/2	0.27	0.013	0.32	0.29
2776.675	26,488	9/2	62,492	7/2	−0.58	0.013	−0.54	−0.69
2788.825	23,833	9/2	59,680	9/2	−1.33	0.010	−1.23	−1.92
2807.753	12,418	5/2	48,023	3/2	−0.38	0.057	−0.33	−0.43
2816.157	13,461	9/2	48,960	11/2	0.51	0.024	0.55	0.54
2842.148	12,034	3/2	47,209	1/2	−0.87	0.021	−0.85	−0.92
2848.233	12,901	7/2	48,000	9/2	0.30	0.027	0.33	0.32
2855.917	24,836	5/2	59,841	3/2	−1.11	0.010	−1.31	−2.53
2866.540	15,428	9/2	50,303	7/2	−1.42	0.037	−1.61	−1.57
2871.512	12,418	5/2	47,232	7/2	0.10	0.010	0.13	0.11
2890.993	12,034	3/2	46,614	5/2	−0.08	0.010	−0.12	−0.14
2894.451	13,461	9/2	48,000	9/2	−0.10	0.009	−0.15	−0.17
2909.116	11,784	1/2	46,148	3/2	−0.50	0.120	−0.47	−0.49
2911.917	12,901	7/2	47,232	7/2	−0.10	0.009	−0.06	−0.07
2913.806	28,989	7/2	63,299	7/2	−0.37	0.016	−0.51	−0.38
2923.391	12,418	5/2	46,614	5/2	−0.12	0.010	−0.08	−0.10
2926.153	28,877	5/2	63,042	5/2	−0.55	0.019	−0.54	−0.75
2930.502	12,034	3/2	46,148	3/2	−0.18	0.031	−0.19	−0.21
2934.297	11,784	1/2	45,853	1/2	−0.40	0.120	−0.36	−0.37
2935.776	28,989	7/2	63,042	5/2	−1.00	0.006	−0.97	−1.25
2938.300	28,989	7/2	63,013	9/2	−0.38	0.008	−0.39	−0.26
2956.056	12,034	3/2	45,853	1/2	−0.77	0.007	−0.91	−0.94
2960.241	13,461	9/2	47,232	7/2	−1.30	0.003	−1.26	−1.28
2963.797	12,418	5/2	46,148	3/2	−0.90	0.011	−0.87	−0.88
2965.280	12,901	7/2	46,614	5/2	−0.96	0.011	−0.97	−0.98
2975.404	29,699	5/2	63,299	7/2	−0.12	0.041	−0.15	−0.05
3030.070	30,020	7/2	63,013	9/2	−1.32	0.009	−1.46	−1.66
3052.322	26,740	11/2	59,492	13/2	−0.65	0.022	−0.69	−0.82
3054.930	29,022	5/2	61,747	3/2	−1.06	0.009	−1.15	−0.82
3078.633	30,020	7/2	62,492	7/2	−1.17	0.058	−1.18	−1.19
3087.620	27,114	13/2	59,492	13/2	0.36	0.028	0.49	0.43
3097.687	26,488	9/2	58,761	11/2	−0.73	0.009	−0.76	−0.81
3111.636	26,069	9/2	58,197	9/2	−0.92	0.018	−1.03	−1.13
3136.466	23,833	9/2	55,707	7/2	−0.55	0.065	−0.53	−0.46
3144.625	26,406	7/2	58,197	9/2	−1.03	0.038	−1.13	−1.29
3158.933	27,114	13/2	58,761	11/2	−1.05	0.006	−0.95	−1.03
3175.051	26,406	7/2	57,892	7/2	−0.27	0.022	−0.16	−0.32
3178.004	26,740	11/2	58,197	9/2	−0.98	0.006	−0.84	−0.94
3183.405	26,488	9/2	57,892	7/2	−0.94	0.022	−0.89	−1.04
3258.677	17,344	5/2	48,023	3/2	−1.47	0.011	−1.48	−1.40
3267.633	25,113	5/2	55,707	7/2	−1.00	0.040	−1.11	−0.81
3292.313	25,342	7/2	55,707	7/2	0.05	0.006	−0.01	0.18
3347.266	24,372	1/2	54,239	1/2	−0.81	0.012	−1.02	−0.70
3367.959	33,046	9/2	62,729	11/2	−0.11	0.011	−0.02	0.14
3374.833	32,124	1/2	61,747	3/2	−1.26	0.030	−1.34	−1.40
3379.755	24,660	3/2	54,239	1/2	−0.81	0.002	−0.91	−0.68
3435.376	30,392	11/2	59,492	13/2	−0.34	0.041	−0.31	−0.44
3445.500	28,877	5/2	57,892	7/2	−0.41	0.013	−0.51	−0.63
3545.989	29,699	5/2	57,892	7/2	−1.03	0.065	−0.96	−1.00
3547.942	30,020	7/2	58,197	9/2	−1.08	0.040	−0.95	−1.00
3618.359	35,100	13/2	62,729	11/2	−1.34	0.021	−1.33	−1.39
3658.959	35,406	11/2	62,729	11/2	−0.76	0.017	−0.77	−0.69
3857.196	24,660	3/2	50,578	5/2	−0.99	0.052	−0.97	−1.41

[a] The wavelengths, given in vacuum (air) below (above) 2000 Å are deduced from the experimental energy level values.

[b] Experimental energy levels taken from [4].

[c] Experimental values deduced from [9,12,13].

[d] Values obtained in the present work using the oscillator strength parametrization (OSP) and core-polarization-corrected relativistic Hartree Fock (HFR+CPOL) methods.

$4d^45d$ and $4d^45p$, $4d^35s5p$ configurations in the even and odd parities, respectively.

As seen from Table 3, the OSP results are in very good agreement with the experimental oscillator strengths, the average ratio gf_{OSP}/gf_{EXP} being equal to 0.98 ± 0.20, where the uncertainty corresponds to the standard deviation to the mean. A similar ratio, i.e. 0.94 ± 0.30, is found when considering the comparison between HFR+CPOL and experimental results, provided that the computed *gf*-values corresponding to transitions affected by strong cancellation effects are rejected from the mean, namely those appearing at $\lambda = 2111.248$, 2113.819, 2122.698, 2187.622, 2515.080, 2618.465, 2747.619, 2855.917, and 3857.196 Å. For these lines, it was indeed observed that the cancellation factor, *CF*, as defined by Cowan [17] took very small values ($CF < 0.05$) in our HFR+CPOL calculations, indicating that the corresponding oscillator strengths could not be reliable.

Finally, in a Supplementary file, we give the oscillator strengths and transition probabilities computed in the present work using the HFR+CPOL method for about 1800 Mo II spectral lines involving available experimental energy levels with calculated log-*gf* values greater than −2. This table covers a wide range of wavelengths, from 1750 to 8700 Å and includes many new radiative parameters, not only for $4d^5$–$4d^45p$ and $4d^45s$–$4d^45p$ transitions, but also for $4d^45s$–$4d^35s5p$ and $4d^35s^2$–$4d^35s5p$ transitions.

4. Conclusion

A new investigation of radiative decay rates for transitions in Mo II using the semi-empirical oscillator strength parametrization approach and the relativistic Hartree Fock method including core-polarization effects is reported in the present work. It is shown that both methods give a similar good agreement when compared to available experimental *gf*-values. It is also observed that the $4d^45s$ $4d^45p$ radial dipole integral deduced from our oscillator strength parametrization approach has a similar value to the one obtained with the HFR+CPOL method. The trend is confirmed when we compare the OSP and HFR+CPOL $nd^k(n+1)s \rightarrow nd^k(n+1)p$ transition radial integrals in the case of other singly ionized atoms, such as Sc II, Ti II, V II, Zr II, Nb II, Rh II and Hf II.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.jqsrt.2017.05.019.

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