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Core-polarization effects in the cadmium isoelectronic sequence

Emile Biémont
Institut d'Astrophysique, Université de Liège, B-4000 Liège, Belgium

Charlotte Froese Fischer
Department of Electrical Engineering and Computer Science, Vanderbilt University, Box 1679 B, Nashville, Tennessee 37235

Michel R. Godefroid
Laboratoire de Chimie Physique Moléculaire, CP160/09, Université Libre de Bruxelles, B-1050 Bruxelles, Belgium

Patrick Palmeri and Pascal Quinet
Astrophysique et Spectroscopie, Université de Mons-Hainaut, B-7000 Mons, Belgium

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The oscillator strengths of the allowed and spin-forbidden $5s^2\ ^1S_0-5s5p\ ^{1,3}P_1^o$ transitions in the cadmium isoelectronic sequence are evaluated for $48 \leqslant Z \leqslant 57$ using the relativistic Hartree-Fock approach, including a core-polarization potential, and the multiconfiguration Dirac-Fock method, taking the valence and core-valence correlation effects into account. A good agreement is noted when comparing the two sets of theoretical data and when comparing theory with experiment for the spin-forbidden transition. The discrepancies observed between theory (both theories being in agreement) and experiment for the singlet-singlet transition indicate that some experimental data are in need of revision.

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I. INTRODUCTION

In recent years, the allowed and spin-forbidden $5s^2\ ^1S_0-5s5p\ ^{1,3}P_1^o$ resonant transitions of the Cd-like ions up to La^{9+} have been the subject of different theoretical and experimental investigations. The lifetimes of the $5s5p\ ^{1,3}P^o$ states were investigated in Cd I with the level crossing technique [1,2], beam-foil spectroscopy [3], the atomic-beam laser-excitation technique [4], and the phase-shift [5] and delayed-coincidence methods [6]. In In II, the experimental results were obtained by laser spectroscopy of In$^+$ ions stored in a radio-frequency trap [7], by beam-foil spectroscopy [8–10], or by the delayed-coincidence method [11]. In the subsequent ions along the isoelectronic sequence, the available data are all beam-foil measurements corrected or not corrected with the arbitrarily normalized decay curve technique [9,12–17]. Some appreciable discrepancies are observed when comparing all these experimental results.

On the theoretical side, some calculations are due to Helliwell [18], who used a nodal stability criterion to calculate wave functions and oscillator strengths, to Hafner and Schwarz [19], who considered a relativistic pseudopotential approach with core-valence correlation, and to O'Neill *et al.* [13], who performed a multiconfiguration Hartree-Fock calculation of the oscillator strength of the resonance transition in the singlet system. In I^{5+}, however, theory and observation in Ref. [13] differ by a factor of 2. Hibbert [20] has carried out a configuration interaction calculation taking valence correlation effects into account. Even when introducing core-polarization effects into the calculations, some persistent discrepancies are observed between experimental and theoretical lifetimes, particularly in the triplet system. Calculations along the cadmium isoelectronic sequence, performed with an approach combining limited relativistic configuration mixing and a polarization model, have been published by Migdalek and Baylis [21]. Further investigations along the same sequence were carried out by Migdalek and Bojara, using the multiconfiguration relativistic Hartree-Fock scheme [22] or the single-configuration relativistic Hartree-Fock technique [23]. Similar discrepancies between theory and experiments were also noted by Chou and Huang [24] when the experimental oscillator strengths for the intercombination and resonance transitions in Cd-like ions were compared with the multiconfiguration relativistic random-phase approximation (MCRRPA) results. These discrepancies are reduced but still remain when a large-scale MCRRPA calculation is performed that includes core-excitation channels [25]. Recent theoretical results are due to Lavín *et al.* [26,27], who applied the relativistic quantum defect orbital method with and without explicit account for core-valence correlation to the singlet-singlet transition, and to Biémont and Zeippen [28], who used the relativistic Hartree-Fock (HFR) approach, taking intravalence configuration interaction and core-polarization effects into account.

In order to give more insight into the problem caused by the disagreement between theory and experiment for several Cd-like ions, and in order to definitely establish whether the persistent discrepancies theory-experiment emphasized in different papers are due to an inadequate theoretical model or to inaccurate experimental measurements, we compare, in the present work, two different and completely *independent* theoretical approaches. Both consider valence correlation and, in addition, core-polarization effects in a detailed way using either a semiempirical or a purely *ab initio* approach. These two methods are the HFR approach and the multiconfiguration Dirac-Fock (MCDF) technique, which are both adequate for heavy ions where relativistic effects are expected to play a major role. The computer facilities available have allowed us to substantially refine the calculations as far as electron correlation is concerned, although the computer time required for the calculations is growing considerably with the number of configurations introduced in the model, particularly in the MCDF approach.

II. COMPUTATIONAL METHODS

A. The HFR method

For the Cd-like ions, accurate calculations of atomic structure should allow for both intravalence and core-valence correlation. Migdalek and Baylis [29] have suggested an approach in which the largest part of the intravalence correlation is represented within a configuration interaction scheme while core-valence correlation is approximated by a core-polarization model potential. For atoms with n valence electrons, the one-particle operator of this potential can be written as

$$V_{P1} = -\tfrac{1}{2}\,\alpha_d \sum_{i=1}^{n} \frac{r_i^2}{(r_i^2 + r_c^2)^3}, \tag{1}$$

where α_d is the dipole polarizability of the core and r_c is the cutoff radius that is arbitrarily chosen as a measure of the size of the ionic core.

In addition, the interaction between the modified electric fields experienced by the valence electrons gives rise to a two-particle term given by

$$V_{P2} = -\alpha_d \sum_{i>j} \frac{\vec{r}_i \cdot \vec{r}_j}{[(r_i^2 + r_c^2)(r_j^2 + r_c^2)]^{3/2}}. \tag{2}$$

A further correction, introduced by Hameed *et al.* [30] and Hameed [31], to allow for more accurate treatment of the penetration of the core by the valence electrons, corresponds in the present formalism to the addition to the integral

$$\int_0^\infty P_{nl}(r)\,\frac{r}{(r^2 + r_c^2)^{3/2}}\,P_{n'l'}(r)\,dr \tag{3}$$

in Eq. (2) of the core-penetration term

$$\frac{1}{r_c^3}\int_0^{r_c} P_{nl}(r)\,r\,P_{n'l'}(r)\,dr. \tag{4}$$

When including the core polarization and core penetration in the Hamiltonian, the dipole-moment operator in the transition matrix element also has to be modified for consistency. The dipole radial integral

$$\int_0^\infty P_{nl}(r)\,r\,P_{n'l'}(r)\,dr \tag{5}$$

has to be replaced by

$$\int_0^\infty P_{nl}(r)\,r\left(1 - \frac{\alpha_d}{(r^2 + r_c^2)^{3/2}}\right)P_{n'l'}(r)\,dr - \frac{\alpha_d}{r_c^3}\int_0^{r_c} P_{nl}(r)\,r\,P_{n'l'}(r)\,dr. \tag{6}$$

TABLE I. Adopted core-polarization parameters in the HFR calculations.

Ion	Z	$\alpha_d(a_0^3)$	$r_c(a_0)$
Cd I	48	5.67	0.980
In II	49	3.65	0.881
Sn III	50	2.48	0.799
Sb IV	51	1.81	0.730
Te V	52	1.38	0.672
I VI	53	1.08	0.621
Xe VII	54	0.86	0.576
Cs VIII	55	0.69	0.537
Ba IX	56	0.56	0.502
La X	57	0.45	0.471

In the present work, the wave functions were obtained by the HFR method [32,33] using Cowan's suite of computer codes, in which we have incorporated the core-polarization and core-penetration corrections as described above. The relative contributions to energy levels and oscillator strengths of these two corrections have been estimated in the ions Cd I and La X. We found that, while the effect on transition energies is very small ($<0.5\%$), the introduction of core-polarization and core-penetration corrections leads to a reduction of the oscillator strengths by an amount of $\sim 30\%$ in both ions, from which $\sim 2\%$ is due to core-penetration effects.

Outer correlation was considered among the configurations $5s^2$, $5sns(n=6-10)$, $5snd(n=5-10)$, $5p^2$, $5d^2$, $4f^2$, $5f^2$, $5p6p$, $5p7p$ for the even parity and $5snp(n=6-10)$, $5p6s$, $5p7s$, $5p5d$, $5p6d$, $5p7d$ for the odd parity. The adopted core-polarization parameters, α_d and r_c, are quoted in Table I. For the dipole polarizabilities, we have used the values reported by Fraga *et al.* [34] for the ions Cd III–La XII, slightly modified to obtain a smooth curve along the sequence. The cutoff radii r_c have been adjusted to match the experimental ionization potentials to within 1%, with the constraint being that the behavior along the sequence is the same as the one obtained for the *ab initio* HFR average values $\langle r \rangle$ of the outermost core orbitals, $4d^{10}$ (see Fig. 1).

The ionization potentials used in this procedure were taken from Moore [35] for the ions Cd I to Sb IV, from Crooker and Joshi [36] for Te V, from Kaufman *et al.* [37] for I VI, and from Kaufman and Sugar [38] for the ions Xe VII to La X. Using a well established least-squares-fitting procedure [33], the values of the average energies $E_{\mathrm{av}}(5s^2)$ and $E_{\mathrm{av}}(5s5p)$ and the Slater integral $G^1(5s,5p)$ have been adjusted to obtain the best agreement between the calculated and the experimental ${}^1S$-${}^1P^o$ and ${}^1S$-${}^3P^o$ transition energies taken from Moore [35] (Cd I, In II, Sn III, Sb IV), Pinnington

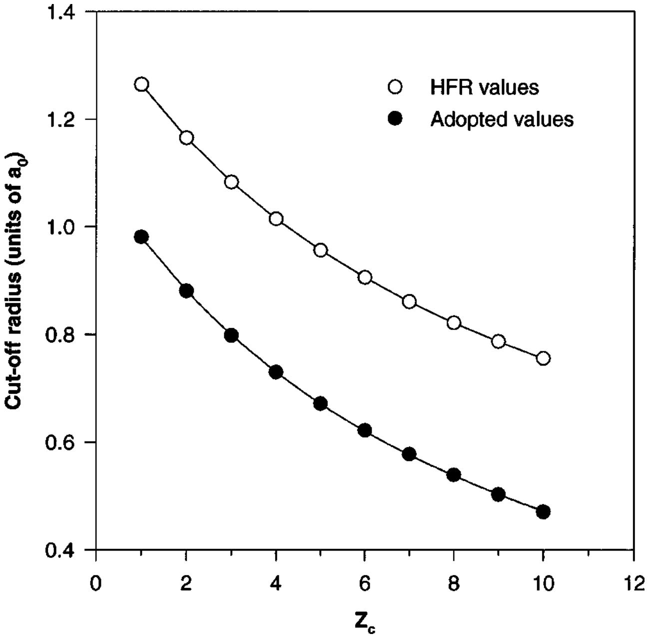

FIG. 1. Cutoff radii (r_c in a_0) for Cd-like ions, used in the core-polarization model. $Z_c = Z - N + 1 = Z - 48 + 1$ for the Cd-like 48-electron system.

et al. [17] (Sb IV), Crooker and Joshi [36] (Te V), Kaufman and Sugar [38] (Xe VII, Ba IX), Gayasov and Joshi [39] (Cs VIII), and Gayasov *et al.* [40] (La X). The other Slater integrals have been scaled down by a factor 0.85 while the *ab initio* values of the spin-orbit parameters have been used without scaling.

B. The MCDF Method

In the multiconfiguration Dirac-Fock method [41], the Hamiltonian is given by

$$\sum_{i=1}^{N}\left[c\boldsymbol{\alpha}_i\cdot\mathbf{p}_i+(\beta_i-1)c^2-\frac{Z}{r_i}\right]+\sum_{i<j}^{N}\frac{1}{r_{ij}}, \tag{7}$$

where c is the speed of light and $\boldsymbol{\alpha}$ and β are the Dirac matrices. The atomic wave functions are given as an expansion over *jj*-coupled configuration state functions (CSFs)

$$|\Psi(JM_J\pi)\rangle=\sum_i c_i|\Phi(\alpha_i JM_J\pi)\rangle. \tag{8}$$

The CSFs in turn are constructed from Slater determinants built on the four-component Dirac orbitals

$$\phi(\mathbf{r})=\frac{1}{r}\begin{pmatrix}P_{n\kappa}(r)\chi_{\kappa m}(\hat{r})\\ iQ_{n\kappa}(r)\chi_{-\kappa m}(\hat{r})\end{pmatrix}. \tag{9}$$

In the expression above, κ is the relativistic angular quantum number, $P_{n\kappa}(r)$ and $Q_{n\kappa}(r)$ are the large and small component radial wave functions, and $\chi_{\kappa m}(\hat{r})$ is the spinor spherical harmonic in the *lsj* coupling scheme

$$\chi_{\kappa m}(\hat{r})=\sum_{m_l,m_s}\langle l\,\tfrac{1}{2}\,m_l m_s|jm\rangle Y_{lm_l}(\theta,\varphi)\xi_{m_s}(\sigma). \tag{10}$$

The radial functions $P_{n\kappa}(r)$ and $Q_{n\kappa}(r)$ are numerically represented on a logarithmic grid and are required to be orthonormal within each κ symmetry. In the MCDF variational procedure, the radial functions *and* the expansion coefficients $\{c_i\}$ are optimized to self-consistency.

We investigated the cadmium isoelectronic sequence by exploring the active space method for building the MCDF multiconfiguration expansion. The latter is produced by exciting the electrons from the reference configuration to a given active set (AS) of orbitals. The rules adopted for generating the configuration space differ according to the correlation model being used. Within a given correlation model, the active set of orbitals spanning the configuration space is increased to monitor the convergence of the total energies and the oscillator strengths of both the allowed and spin-forbidden transitions.

The notation for the active sets consists of the pair of the maximum principal and orbital quantum numbers $(nl)_{\max}$ considered in the orbital set used for building the configuration space. In this connection, since the principal quantum number of virtual or correlation orbitals has no significance in our method, and since it was convenient to treat the core as having orbitals with principal quantum number $n\leqslant 4$, the $4f$ orbital was inactive (i.e., ignored) in our approach. Two *ab initio* models have been investigated. In the first model, *valence correlation* (V) is described by MCDF expansions involving single and double excitations (SD) from $5s^2\ ^1S_0$ and $5s5p\ ^{1,3}P_1^o$ for even and odd parity, respectively, to the $(nl)_{\max}=5g$ and $6g$ active sets. These calculations are labeled MCDF-V($5g$) and MCDF-V($6g$).

The ‘‘optimal level’’ (OL) model has been selected, choosing the lowest eigenpair of $^1S_0$ symmetry and the second root for the $^1P_1^o$ symmetry. For the $^3P_J^o$ symmetry, we selected an ‘‘extended optimal level’’ (EOL) model where the three atomic state functions ($J=0,1,2$) are assigned their statistical weight ($2J+1$). In the MCDFV($5g$) calculations, all orbitals were optimized variationally. When adding an extra layer ($6g$), the orbitals up to $n=5$ were taken from the corresponding MCDFV($5g$) calculation and only the last nine orbitals $6l_{j=l\pm 1/2}$ corresponding to $0\leqslant l\leqslant 4$ were variational.

In a more elaborate model, *core-valence correlation* (CV) is also included by considering SD-core-valence excitations from $4d^{10}5s^2\ ^1S_0$ and $4d^{10}5s5p\ ^{1,3}P_1^o$ for even and odd parity, respectively. These calculations are labeled MCDFCV(AS), where the orbital active set is specified by $(nl)_{\max}$, as described above. The $5f$, $6f$, and $7f$ active sets have been considered, with the additional constraint that a maximum of one hole is created in the $4d$ subshell. The $n=4$ radial wave functions were taken from the valence correlation MCDFV($5g$) calculation for the three $LS\pi$ symmetries, and kept frozen in the variational procedure. Only the $n=5$ orbitals are optimized, using the OL/EOL model as

TABLE II. Comparison of MCDF excitation energies, $\Delta E_{\mathrm{theor}}$, with experiment, ΔE_{expt} (in cm^{-1}).

		$5s^2\ ^1S_0$-$5s5p\ ^3P_1^o$		$5s^2\ ^1S_0$-$5s5p\ ^1P_1^o$	
Ion	Z	$\Delta E_{\mathrm{theor}}$	ΔE_{expt}[a]	$\Delta E_{\mathrm{theor}}$	ΔE_{expt}[a]
Cd I	48	30 818	30 656	43 512	43 692
In II	49	43 655	43 349	62 714	63 034
Sn III	50	55 646	55 196	79 538	79 911
Sb IV	51	67 283	66 700	95 566	95 956
Te V	52	78 737	78 025	111 313	111 708
I VI	53	90 095	89 262	127 037	127 424
Xe VII	54	101 403	100 451	142 889	143 261
Ca VIII	55	112 700	111 628	158 984	159 326
Ba IX	56	124 003	122 812	175 402	175 711
La X	57	135 123	134 020	192 218	192 481

[a] From Ref. [35] (Cd I to Sb IV), Ref. [36] (Te V), Ref. [37] (I VI), and Ref. [38] (Xe VII to La X).

described above. When further extending the active set to $6f$ and $7f$, only the orbitals of the last layer were variational. For the MCDFCV($7f$) calculation of $^3P_1^o$, however, the OL optimization model has been chosen instead of the EOL in order to limit the size of the expansion, which still reaches 7404 relativistic CSFs. This rather large calculation has been performed only for the heaviest ion considered in the present work, i.e., $\mathrm{La}^{9+}(Z=57)$, due to the extensive computer resources that it requires (more than 12 h of CPU time using eight parallel processors on a Silicon Graphics Origin 2000).

III. DISCUSSION

The *ab initio* MCDFCV excitation energies and fine-structure splittings corresponding to the largest active sets are reported and compared with observation in Tables II and III, respectively. The agreement is quite satisfactory, to within 1% for the ΔE_{th} of Table II and 4% for the CV($n=6f$) calculation of Table III. As illustrated in Fig. 2 (dotted line), the excitation energies obtained at the valence correlation level of approximation are systematically too low. Core-polarization effects are large indeed, and their inclusion is essential to get close agreement between theory and experiment.

The oscillator strengths for the spin-forbidden and the allowed $5s^2\ ^1S_0-5s5p\ ^{3,1}P_1^o$ electric-dipole transitions, calculated using the Coulomb (C) and Babushkin (B) gauges [42] in the MCDF approximation, are displayed in Fig. 3 and 4, respectively, for the different correlation models, together with the HFR results. The experimental oscillator strength values, with their error bars, are shown when available.

The theoretical oscillator strengths calculated in the present work using both the HFR and MCDF methods are reported in Table IV for the spin-forbidden and the allowed $5s^2\ ^1S_0-5s5p\ ^{3,1}P_1^o$ electric-dipole transitions. In the MCDF approach, the comparison is limited to the most complete core-valence calculations, i.e., MCDFCV($6f$) or MCDFCV($7f$). They are compared with other theories in the same table. The reported MCDF radiative data have been calculated using the experimental transition energies to avoid error compensation in the theoretical line strength and energy factors.

A. The singlet-triplet transition

Figure 3 shows the change in the oscillator strength as more correlation is added as a function of the nuclear charge Z. Note the excellent agreement in the gauges for the valance correlation calculation, but that Fig. 2 showed the transition energies to be in considerable error. It is clear that agreement between gauges alone does not guarantee the accuracy of oscillator strengths. As more core polarization is included, the oscillator strength increases, particularly for higher Z. This can be expected since f orbitals become increasingly

TABLE III. Comparison of *ab initio* MCDF and observed fine-structure splittings of $5s5p\ ^3P^o$ (in cm^{-1}).

Ion	Z	J-J'	V($6g$)	CV($5f$)	CV($6f$)	Expt.
Cd I	48	1-0	480	512	523	542.113
		2-1	1483	1088	1126	1170.866
In II	49	1-0	1017	1034	1041	1074
		2-1	2242	2349	2395	2478
Sn III	50	1-0	1613	1603	1605	1648.4
		2-1	3728	3860	3918	4032.2
Sb IV	51	1-0	2261	2214	2208	2265
		2-1	5477	5644	5714	5860
Te V	52	1-0	2961	2863	2850	2915
		2-1	7510	7724	7810	7981
I VI	53	1-0	3709	3549	3525	3596
		2-1	9855	10 128	10 232	10 423
Xe VII	54	1-0	4503	4265	4231	4311
		2-1	12 538	12 884	13 007	13 223
Cs VIII	55	1-0	5339	5010	4964	5054
		2-1	15 591	16 023	16 167	16 403
Ba IX	56	1-0	6215	5780	5720	5821
		2-1	19 044	19 576	19 740	20 000
La X	57	1-0	7125	6572	6499	6613
		2-1	22 932	23 577	23 766	24 046

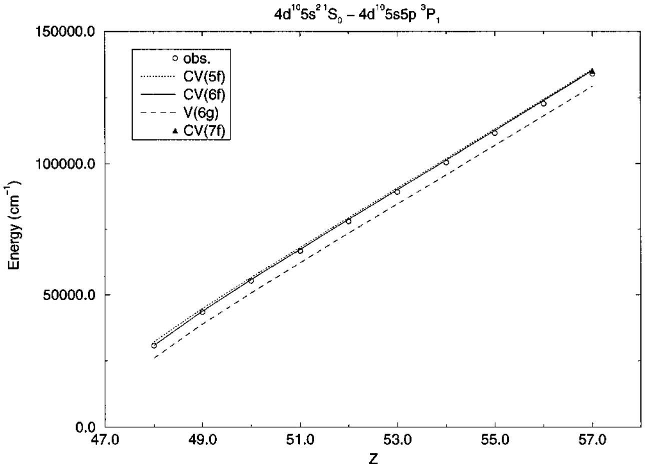

FIG. 2. Excitation energies (in cm^{-1}) of $5s5p\ ^3P_1^o$ of Cd-like ions.

important. It appears that the calculations may not have converged, that more layers may be needed, but the one calculation that also includes the $n=7$ layer of orbitals has excellent agreement in gauges, and lies *between* the Coulomb and Babushkin values of the previous calculation. As can be seen from both Table IV and Fig. 3, the MCDF f values corresponding to the most complete correlation model [CV($6f$) or CV($7f$)] are systematically higher than the HFR results. The largest relative difference occurs for Cd I, even if this cannot be realized from the figure because of its scale. Except for neutral cadmium, the relative difference between MCDF and HFR never exceeds 15%, and it occurs when the Coulomb gauge is selected for the MCDF approach.

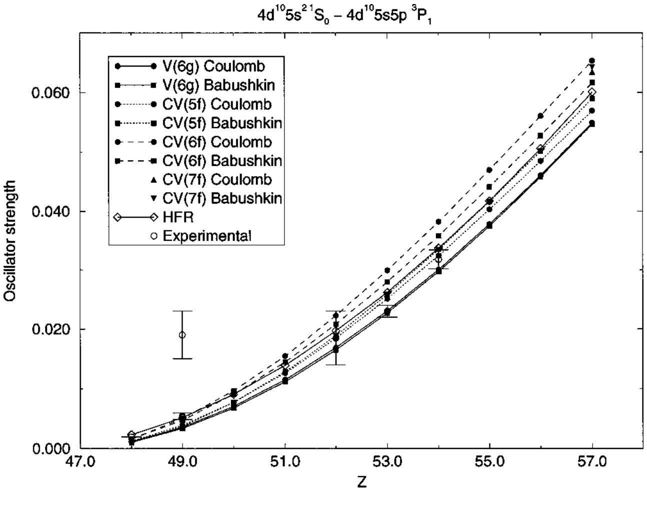

FIG. 3. Oscillator strengths of $5s^2\ ^1S_0$-$5s5p\ ^3P_1^o$ in Cd-like ions. The experimental values (with error bars) are taken from the following sources: Cd I ($Z=48$), [2]; In II ($Z=49$), low value [7], high value [8]; Te V ($Z=52$), [43]; I VI ($Z=53$), [13]; Xe VII ($Z=54$), [14].

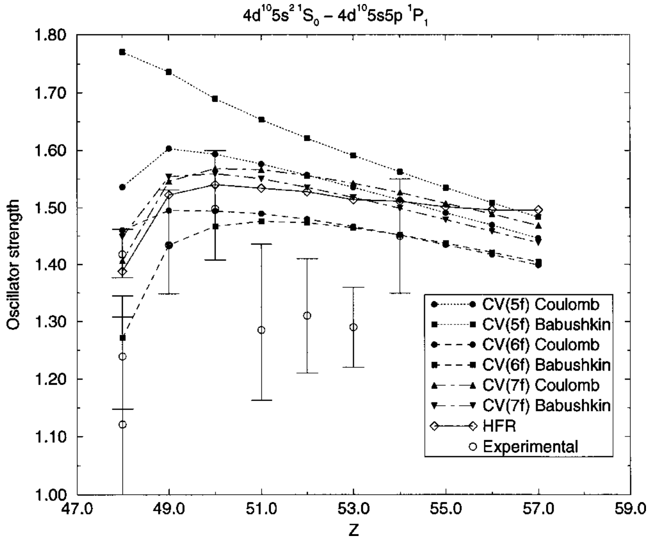

FIG. 4. Oscillator strengths of $5s^2\ ^1S_0$-$5s5p\ ^1P_1^o$ in Cd-like ions. The experimental values (with error bars) are taken from the following sources: Cd I ($Z=48$), [1,3,5]; In II ($Z=49$), [10]; Sn III ($Z=50$), [12]; Sb IV ($Z=51$), [17]; Te V ($Z=52$), [44]; I VI ($Z=53$), [15]; Xe VII ($Z=54$), [44].

For $\mathrm{In}^+(Z=49)$, our theoretical calculations together with the radio-frequency trap laser spectroscopy measurement of Peik *et al.* [7] definitely invalidate the beam-foil result of Andersen *et al.* [8]. The f values of Ref. [28], both for the singlet-triplet and the singlet-singlet transitions, are somewhat larger than the results obtained in the present work, but it should be emphasized that Ref. [28] was a large-scale calculation that did not specifically focus on the two transitions considered here. Figure 3 shows that the agreement with observation [43] is rather good for $\mathrm{Te}^{4+}(Z=52)$. For higher nuclear charges (I^{5+},Xe^{6+}), the experimental accuracy looks overestimated [13,14]. Experimental work would be very welcome for $Z=55-57$ for assessing the reliability of the present theoretical work in that range.

B. The singlet-singlet transition

The oscillator strengths of $5s^2\ ^1S_0-5s5p\ ^1P_1^o$ are displayed in Fig. 4. The MCDF results now exhibit an oscillator behavior as more correlation orbitals are added. The $n=7$ Coulomb and Babushkin results now define a narrow band that lies between those for $n=5$ and $n=6$. As it also appears in Table IV, the agreement between the most elaborate MCDF calculations [MCDFCV($7f$)] and HFR results is rather satisfactory. The corresponding f values are systematically lower than the gauge independent multiconfiguration relativistic random-phase approximation (MCRRPA) results of Chou *et al.* [25] (which are not displayed in the figure but given in Table IV).

For neutral cadmium, the MCDFCV($7f$) and HFR results support the large oscillator strength [$f=1.42(4)$] derived from the old level crossing lifetime measurement of Lurio and Novick [1] against the smaller f values obtained from the phase-shift [5] or beam-foil [3] lifetime measurements. The present theoretical work has improved on the whole the theory-experiment agreement along the sequence, but the even cascade-corrected experimental results from Pinnington and co-workers [12,44,15] are definitely too low for Sb^{3+}, Te^{4+} and $\mathrm{I}^{5+}(Z=51-53)$.

TABLE IV. Comparison of HFR and MCDF-CV oscillator strengths of $5s^2\ ^1S_0-5s5p\ ^{3,1}P_1^o$ with other theories.

		Present work			Other theory					
	Z	HFR	MCDFCV[a]		CIV3[b]	MCDF+POL[c]	CIRHF+CP[d]	MCRRPA[e]	RQDO+POL[f]	HFR[g]
Ion			C	B						
$5s^2\ ^1S_0-5s5p\ ^3P_1^o$										
Cd I	48	0.002 32	0.001 67	0.001 64	0.0027	0.001 25	0.008 11	0.001 304		
In II	49	0.005 19	0.005 07	0.004 71	0.0064	0.003 25	0.006 03	0.004 00		0.0073
Sn III	50	0.009 04	0.009 94	0.008 96		0.005 99	0.008 72	0.007 90		
Sb IV	51	0.0139	0.0156	0.0143		0.009 51	0.012 85	0.012 87		
Te V	52	0.0197	0.0225	0.0206		0.0137	0.0185	0.018 80		
I VI	53	0.0262	0.0302	0.0277	0.019	0.0187	0.0244	0.025 54		
Xe VII	54	0.0337	0.0386	0.0355	0.030	0.0241	0.0301			
Cs VIII	55	0.0417	0.0474	0.0437		0.0301	0.0370			
Ba IX	56	0.0506	0.0566	0.0523		0.0367	0.0445			
La X	57	0.0601	0.0639	0.0638						
$5s^2\ ^1S_0-5s5p\ ^1P_1^o$										
Cd I	48	1.388	1.401	1.455	1.764	1.355	1.35		1.19	
In II	49	1.522	1.538	1.562	2.204	1.578	1.57		1.44	1.636
Sn III	50	1.540	1.561	1.567		1.609	1.60	1.748	1.46	
Sb IV	51	1.534	1.560	1.557		1.615	1.62	1.717	1.40	
Te V	52	1.528	1.551	1.541		1.626	1.57	1.685	1.39	
I VI	53	1.514	1.538	1.523	2.174	1.614	1.57	1.655	1.33	
Xe VII	54	1.511	1.523	1.503	2.154	1.600	1.57	1.626	1.36	
Cs VIII	55	1.501	1.504	1.482		1.700	1.60		1.35	
Ba IX	56	1.496	1.486	1.461		1.703	1.61		1.33	
La X	57	1.496	1.467	1.440						

[a] CV($7f$) for the singlet-singlet transition in all ions. CV($6f$) for the singlet-triplet transition in all ions but La^{+9} [CV($7f$)] (C and B stand for the Coulomb and Baushkin gauges, respectively).

[b] Hibbert [20].

[c] Migdalek and Baylis [21].

[d] Migdalek and Bojara [23].

[e] Chou *et al.* [25].

[f] Lavín *et al.* [26].

[g] Biémont and Zeippen [28].

C. Comparison of lifetimes

The HFR and MCDF lifetimes of $5s5p\ ^{1,3}P_1^o$ are compared in Table V with the available experimental values and with the semiempirical predictions of Curtis [45] made in the context of a data-based isoelectronic parametrization. For the $5s5p\ ^1P_1^o$ lifetimes, the agreements between the two approaches and between the Coulomb and Babushkin results within the MCDF approach are almost perfect, supporting the validity of the theoretical results.

The $5s5p\ ^3P_1^o$ lifetimes are obviously more difficult to evaluate than those of the singlet states. In the MCDF method, the largest difference between the Coulomb and Babushkin formalisms occurs for Sn III (11.5%). For this ion and higher nuclear charges ($Z \geqslant 50$), the Babushkin gauge gives a systematically better agreement with the HFR results. As mentioned above, the comparison for neutral cadmium Cd I reveals a large difference between HFR and MCDF. Most of the experimental lifetimes are between the two theoretical sets.

IV. CONCLUSION

Experimental and theoretical values for the oscillator strengths of the $5s^2\ ^1S_0-5s5p\ ^{1,3}P_1^o$ transitions and for the lifetimes of the $5s5p\ ^{1,3}P_1^o$ levels in the Cd isoelectronic sequence have been examined in the context of the evaluation of the importance of core-polarization effects. Regularities along the sequence and coherence among the HFR and MCDF results have been used to identify erroneous or inaccurate measurements. The predictive power of the two methods for heavy ions such as those considered here is definitively established from their high degree of convergence, provided configuration interaction is considered in the calculations in a sufficiently extensive way and from the good agreement that is observed when comparing theory with the most accurate experimental measurements presently available. Further refinements in the future of the theoretical results cannot be ruled out but are presently excluded basically by the computer capabilities.

TABLE V. Lifetimes (in ns) for the $5s5p\ ^{1,3}P_1^o$ levels in Cd-like ions. For the MCDF results, (C/B) stands for (Coulomb/Babushkin).

Ion	Level	HFR	MCDF (C/B)	Experimental or empirical estimates
Cd I	$^1P_1^o$	1.70	1.68/1.62	1.66±0.05,[a] 1.9±0.15,[b] 2.1±0.3,[c] 1.554[d]
	$^3P_1^o$	2065	2869/2914	2390±40,[e] 2420±60,[f] 2490±130,[g] 2500±250,[h] 2140±60,[i] 2050±50,[j] 2180±70,[k] 2391[d]
In II	$^1P_1^o$	0.74	0.736/0.725	0.90±0.08,[l] 0.79±0.05,[m] 0.760[d]
	$^3P_1^o$	462	472/508	125±25,[n] 440±40,[o] 566[d]
Sn III	$^1P_1^o$	0.46	0.451/0.450	0.54±0.10,[l] 0.47±0.03,[p] 0.52±0.05,[q] 0.490[d]
	$^3P_1^o$	163	148/165	196[a]
Sb IV	$^1P_1^o$	0.32	0.313/0.314	0.56±0.06,[l] 0.38±0.04,[r] 0.349[d]
	$^3P_1^o$	72.9	64.8/70.6	85.2[d]
Te V	$^1P_1^o$	0.24	0.232/0.234	0.41±0.06,[l] 0.260±0.25,[s] 0.28±0.02,[t] 0.263[d]
	$^3P_1^o$	37.6	32.9/35.8	40±10,[s] 42.8[d]
I VI	$^1P_1^o$	0.18	0.180/0.182	0.25±0.03,[u] 0.215±0.012,[v] 0.206[d]
	$^3P_1^o$	21.5	18.7/20.4	24.4±1.2,[u] 23.8[d]
Xe VII	$^1P_1^o$	0.15	0.144/0.146	0.18±0.01,[w] 0.15±0.01,[t] 0.165[d]
	$^3P_1^o$	13.2	11.6/12.6	14.0±0.7,[w] 14.3[d]
Cs VIII	$^1P_1^o$	0.12	0.118/0.120	0.134[d]
	$^3P_1^o$	8.6	7.6/8.3	9.11[d]
Ba IX	$^1P_1^o$	0.10	0.098/0.100	0.111[d]
	$^3P_1^o$	5.9	5.3/5.7	6.10[d]
La X	$^1P_1^o$	0.08	0.083/0.084	0.094[d]
	$^3P_1^o$	4.2	3.9/3.9	4.24[d]

[a] Lurio and Novick [1].
[b] Andersen and Sorensen [3].
[c] Baumann and Smith [5].
[d] Semiemprical predictions of Curtis [45].
[e] Byron *et al.* [2].
[f] van der Veer *et al.* [4].
[g] Schaefer [6].
[h] Koenig and Ellett [46].
[i] Webb and Messenger [47].
[j] Matland [48].
[k] Geneux and Wanders-Vincenz [49].
[l] Andersen *et al.* [9].
[m] Ansbacher *et al.* [10].
[n] Andersen and Sorensen [8].
[O] Peik *et al.* [7].
[p] Pinnington *et al.* [12].
[q] Kernahan *et al.* [16].
[r] Pinnington *et al.* [17].
[s] Pinnington *et al.* [43].
[t] Deduced from the *f* values published by Pinnington *et al.* [44].
[u] O'Neill *et al.* [13].
[v] Ansbacher *et al.* [15].
[w] Kernahan *et al.* [14].

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