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ONE-ELECTRON SPECTRUM OF Yb^+: RELATIVISTIC ENERGIES, TRANSITION PROBABILITIES AND DIPOLE POLARIZABILITY†

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Abstract—Calculations are reported of relativistic ionization energies and transition probabilities in the one-electron spectrum of singly-ionized ytterbium. The relativistic model potential approach used takes into account both valence-core electron exchange and correlation. The influence of polarization of the core by valence electrons on ionization energies and transition probabilities has been studied. Strong cancellation effects have been found for higher transitions of the principal series; these affect both transition probabilities and relative line strengths. The energies are predicted for some states which have not yet been experimentally localized. The static dipole polarizability for Yb^+ is estimated to be 48.18 a_0^3 from computed oscillator strengths; this estimate is compared with lower bounds determined from experimental data.

INTRODUCTION

Numerous experimental studies have been performed on rare earth spectra in different stages of ionization. The objectives have been to measure and assign energy levels and to determine transition probabilities, lifetimes and types of electron coupling. Theoretical studies of rare earths are scarce because of the great complexity of these systems and agreement between theoretical and experimental data is rarely satisfactory. However, for some of the rare earth systems (e.g. Yb(II), Lu(III)), a simple one-electron spectrum, arising from the excitation of an electron out of the $4f$ shell, appears to be superimposed on the complex three-electron spectra. The one-electron spectrum of Yb^+ has been studied by Kaufman and Sugar[1] and the lifetimes of the two lowest $^2P_{1/2,\,3/2}$ states have been measured by several workers.[2-4] We have recently studied[5] the $6s\ ^2S_{1/2}$–$6p\ ^2P_{1/2,\,3/2}$ transitions in Yb(II), for which no other theoretical data appear to exist.

The aim of the present study is to extend the theoretical predictions for the one-electron spectrum of singly ionized ytterbium beyond the lowest levels and transitions treated in the previous paper.[5] We predict, within the single-configuration scheme, the position of the $9s\ ^2S_{1/2}$ state which could not be localized by Kaufman and Sugar,[1] as well as the position of some of the more highly excited states that have not yet been studied. Transition probabilities are also studied for different spectral series. Since our previous study demonstrated a considerable influence of valence-core electron correlation and the resulting polarization of the core, such correlation is included in computations. Because of the numerous calculations required, the relativistic Hartee–Fock method, with the core polarization employed by us,[5] is not used in the present investigations; its use is time consuming even with fast computer facilities. Instead, we have employed the relativistic model potential approach, which gives results very close to those of the single-configuration relativistic Hartree–Fock scheme.[6]

CALCULATIONS

The relativistic model-potential approach is a modification of the semiempirical treatment suggested previously by the author.[7] In order to determine the relativistic wavefunction, the Dirac equations are solved for the valence electron with effective potential

$$V(r) = -\frac{Z}{r} + \frac{1}{r}\int_0^r \rho_c(r_1)\,dr_1 + \int_r^\infty \frac{\rho_c(r_1)}{r_1}\,dr_1 + V_{ex}(r) + V_{pol}(r), \qquad (1)$$

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where

$$V_{ex}(r) = -\frac{1}{r}\left[\frac{6r\rho_c(r)}{\pi^2}\right]^{1/3} F(r),\ F(r) = \frac{1}{2}e^{-r/r_1} \tag{2}$$

and

$$V_{pol}(r) = -\alpha_c r^2/2(r_0^2 + r^2)^3; \tag{3}$$

α_c is the static dipole polarizability of the core and r_0 is the cut-off radius.

The parent-ion density obtained with the relativistic Hartree–Fock code of Desclaux[8] was used as the radial density distribution of the core electrons $\rho_c(r)$. The mean radius of the outermost orbital of the core was adopted as the cut-off radius. Two values of core polarizability α_c were employed: the first is the value computed by Fraga *et al.*[9] in the Hartree–Fock approximation ($\alpha_c = 7.36\ a_0^3$) and the second was found previously by the author[5] under the assumption that the core-polarization-corrected valence electron energies should match experimental ionization energies ($\alpha_c = 11.14\ a_0^3$). The adjustable parameter r_1 was determined in such a way that it matched the model potential valence electron energies for the lowest state of given symmetry to the measured ionization energies reported by Kaufman and Sugar.[1] The resulting values of r_1 were then used for higher states of the same symmetry. The values of the parameters employed in this study are listed in Table 1.

Relativistic transition probabilities have been computed in the long wavelength approximation using the dipole length form.[10] The excitation energies were taken from experiments.[1] When core-polarization effects are included, the dipole-moment operator $\boldsymbol{d} = -\boldsymbol{r}$ of the valence electron in the transition matrix element is replaced by $\boldsymbol{d} + \boldsymbol{d}_c$, where $\boldsymbol{d}_c$ is the dipole moment induced in the core by the valence electron, viz.

$$\boldsymbol{d}_c = \alpha_c \boldsymbol{r}(r^2 + r_0^2)^{-3/2}. \tag{4}$$

Four types of computation have been performed. In the first type (RMP = relativistic model potential), core polarization has been completely neglected. The next two types include core

Table 1. Parameters used in different types of calculations. For a description of the calculations and parameters, see the text.

Calculations	State	α_c	r_o	r_1
RMP	s			3.989
	p	-	-	4.665 , 5.683 †
	d			4.825 , 4.977
	f			5.588 , 5.940
RMP + CP Ia	s			2.396
	p			2.674 , 3.115
	d	7.36	1.436	2.793 , 2.862
	f			3.136 , 3.430
RMP + CP Ib	s			1.866
	p			2.045 , 2.369
	d	11.14	1.436	2.190 , 2.239
	f			2.542 , 2.795
RMP + CP II	s		1.000	1.508
	p		2.190	3.603 , 4.285
	d	7.36	1.010	1.700 , 1.759
	f		1.880	3.861 , 4.323

† When two entries are given, the first refers to the $j = \ell - \frac{1}{2}$ state and the second to the $j = \ell + \frac{1}{2}$.

polarization but differ by the value of the core polarizability, which is 7.36 a_0^3 and 11.14 a_0^3 for RMP + CPIa and Ib, respectively. Finally, with RMP + CPII, the value 7.36 a_0^3 is used but the cut-off radius is determined separately for states of different angular quantum number l. The criterion was minimization of the rms deviation between the theoretical and experimental energies of the few lowest states.

DISCUSSION OF RESULTS

(a) *Ionization energies*

The computed valence electron ionization energies† are given in Table 2. For the first three calculations (RMP, RMP + CP Ia,b), the maximum discrepancies between computed and experimental energies are similar and amount to less than 0.5, 4, 2, and 0.5% for s, p, d, and f states, respectively. Adjustment of the cut-off parameter (RMP + CP II) lowers the maximum discrepancy for s states below 0.15% and for d states to 1.1% but does not improve the agreement for f and p states, the latter being the most strongly perturbed. Within the single-configuration approximation, the RMP + CP II computation localizes the $9s\ ^2S_{1/2}$ state, which was not found by Kaufman and Sugar,[1] at $81909 \pm 150\ cm^{-1}$ above the ground $6s\ ^2S_{1/2}$ state. Even if the core polarization is not explicitly included in the effective potential, the

Table 2. Comparisons of computed and measured ionization energies in atomic units. For a description of different types of calculations, see the text.

State	RMP	RMP+CP Ia	RMP+CP Ib	RMP+CP II	Experimental Data[1]
$6s_{1/2}$	0.447747	0.447747	0.447747	0.447747	0.447747
$7s_{1/2}$	0.199354	0.199812	0.199967	0.200390	0.200318
$8s_{1/2}$	0.114389	0.114536	0.114569	0.114821	0.114954
$9s_{1/2}$	0.074322	0.074385	0.074394	0.074541	-
$10s_{1/2}$	0.052189	0.052222	0.052225	0.052315	0.052401
$11s_{1/2}$	0.038667	0.038686	0.038687	-	-
$12s_{1/2}$	0.029799	0.029811	0.029812	-	-
$13s_{1/2}$	0.023668	0.023676	0.023676	-	-
$14s_{1/2}$	0.019249	0.019256	0.019256	-	-
$6p_{1/2}$	0.324444	0.324444	0.324444	0.324444	0.324444
$6p_{3/2}$	0.309269	0.309269	0.309269	0.309269	0.309269
$7p_{1/2}$	0.159917	0.160056	0.160047	0.159947	0.157480
$7p_{3/2}$	0.154772	0.154902	0.154901	0.154789	0.148878
$8p_{1/2}$	0.096475	0.096509	0.096483	0.096453	-
$8p_{3/2}$	0.094059	0.094095	0.094076	0.094036	-
$9p_{1/2}$	0.064678	0.064688	0.064668	0.064656	-
$9p_{3/2}$	0.063346	0.063359	0.063344	0.063325	-
$10p_{1/2}$	0.046407	0.046410	0.046397	0.046391	-
$10p_{3/2}$	0.045596	0.045600	0.045590	0.045579	-
$11p_{1/2}$	0.034930	0.034931	0.034921	-	-
$11p_{3/2}$	0.034399	0.034400	0.034393	-	-
$12p_{1/2}$	0.027245	0.027246	0.027239	-	-

†In the approximation applied in this study, Koopmans' theorem[12] is satisfied and the one-electron valence energies may be interpreted as theoretical ionization energies for the valence electron.

Table 2 (*Contd*).

State	RMP	RMP+CP Ia	RMP+CP Ib	RMP+CP II	Experimental Data[1]
$12p_{3/2}$	0.026879	0.026880	0.026874	-	-
$13p_{1/2}$	0.021845	0.021845	0.021841	-	-
$13p_{3/2}$	0.021581	0.021582	0.021578	-	-
$5d_{3/2}$	0.343130	0.343130	0.343130	0.343130	0.343130
$5d_{5/2}$	0.336870	0.336870	0.336870	0.336870	0.336870
$6d_{3/2}$	0.162827	0.163462	0.163723	0.164558	0.164461
$6d_{5/2}$	0.161223	0.161831	0.162075	0.162920	0.162707
$7d_{3/2}$	0.097922	0.098154	0.098240	0.098695	0.099109
$7d_{5/2}$	0.097188	0.097413	0.097494	0.097958	0.098384
$8d_{3/2}$	0.065510	0.065621	0.065660	0.065922	0.065744
$8d_{5/2}$	0.065110	0.065218	0.065255	0.065524	0.064942
$9d_{3/2}$	0.046928	0.046990	0.047011	0.047174	0.047678
$9d_{5/2}$	0.046684	0.046746	0.046766	0.046932	0.046876
$10d_{3/2}$	0.035276	0.035314	0.035327	-	0.035788
$10d_{5/2}$	0.035117	0.035155	0.035166	-	0.035309
$11d_{3/2}$	0.027486	0.027512	0.027521	-	0.027778
$11d_{5/2}$	0.027377	0.027402	0.027410	-	0.027563
$12d_{3/2}$	0.022020	0.022038	0.022045	-	-
$12d_{5/2}$	0.021942	0.021960	0.021966	-	-
$13d_{3/2}$	0.018034	0.018047	0.018052	-	-
$13d_{5/2}$	0.017976	0.017990	0.017993	-	-
$5f_{5/2}$	0.126512	0.126512	0.126512	0.126512	0.126512
$5f_{7/2}$	0.126160	0.126160	0.126160	0.126160	0.126160
$6f_{5/2}$	0.081078	0.081013	0.081032	0.081046	0.081149
$6f_{7/2}$	0.080919	0.080894	0.080927	0.080943	0.081090
$7f_{5/2}$	0.056268	0.056216	0.056228	0.056240	0.056366
$7f_{7/2}$	0.056180	0.056159	0.056181	0.056196	0.056329
$8f_{5/2}$	0.041299	0.041261	0.041270	0.041278	0.041431
$8f_{7/2}$	0.041244	0.041229	0.041244	0.041255	0.041388
$9f_{5/2}$	0.031591	0.031564	0.031570	0.031577	0.031685
$9f_{7/2}$	0.031554	0.031542	0.031553	0.031560	0.031701

adjustable exchange potential makes partial allowance for this effect.[10] Therefore, explicit inclusion of core polarization through the potential of Eq. (3) results in small changes in ionization energies. The changes are largest for the lowest states of given symmetry and decrease sharply for higher states where the coulombic nature of the effective potential becomes dominant. Their magnitudes are similar for *s*, *p*, and *d* states but much smaller for *f* states.

(b) *Fine-structure splittings*

In Table 3, the fine structure splittings for p, d and f states, calculated as the differences between the one-electron valence energies (the core remains unchanged for different fine-structure states) in $j = l + (1/2)$ and $j = l - (1/2)$ states, are presented. It is seen that, except for the states with lowest n for which the energies were adjusted to match the experimental data, satisfactory agreement occurs only for $6d$, $7d$, and $7f$ states. This result confirms the observation deduced by Kaufman and Sugar[1] from irregularities in the quantum defect curves that the entire np series is perturbed, whereas for nd and nf series the perturbation is more localized. For nd series, it affects mainly states with $n = 8$–11 (although in our results the $6d$ state also seems to be slightly affected) and leads to increasing fine-structure splittings for the $8d$ and $9d$ states. Kaufman and Sugar suggest that the perturber is localized between the $7d$ and $8d$ states. However, as may be seen from Table 3, the fine structure of the $7d$ state is not perturbed. Comparison of the fine-structure splittings obtained with and without core polarization shows that the influence of core polarization is weak for p and d states and that it does not affect the discrepancies between calculations and experiments. However, for the f states, the core polarization decreases these discrepancies considerably. This result is surprising if we recall that the effect of core polarization on energies is larger for p and d states than for f states, but these effects largely cancel for p and d fine-structure splittings.

Table 3. Comparison of calculated and measured fine structure splittings in cm^{-1}.

State	RMP	RMP+CP Ia	RMP+CP Ib	RMP+CP II	Experimental Data [1]
6p	3330.5	3330.5	3330.5	3330.5	3330.41
7p	1129.2	1131.2	1129.4	1132.0	1887.85
8p	530.3	529.8	528.3	530.5	-
9p	292.3	291.7	290.6	292.1	-
10p	178.0	177.8	177.1	178.2	-
11p	116.5	116.5	115.9	-	-
12p	80.3	80.3	80.1	-	-
13p	57.9	57.7	57.7	-	-
5d	1373.9	1373.9	1373.9	1373.9	1373.89
6d	352.0	358.0	361.7	359.5	384.92
7d	161.1	162.6	163.7	161.8	159.10
8d	87.8	88.4	88.9	87.4	176.12
9d	53.6	53.6	53.8	53.1	176.08
10d	34.9	34.9	35.3	-	105.13
11d	23.9	24.1	24.4	-	-
12d	17.1	17.1	17.3	-	-
13d	12.7	12.5	12.9	-	-
5f	77.3	77.3	77.3	77.3	77.29
6f	34.9	26.1	23.0	22.6	12.95
7f	19.3	12.5	10.3	9.7	8.07
8f	12.1	7.0	5.7	5.0	9.59
9f	8.1	4.8	3.7	3.7	-3.45

Table 4. Transition probabilities in s^{-1} and relative line strengths calculated in different types of computation. The notation 1.86E8 corresponds to 1.86×10^8. The statistical (relative line strengths calculated with the spin-orbit interaction neglected) are 1:2 for the principal and sharp series ($s - p$), 5:1:9 for the diffuse ($p - d$) series, and 14:1:20 for the fundamental ($d - f$) series, respectively.

Transition	J - J	Transition Probabilities			Relative line strengths		
		RMP	RMP+CP Ia	RMP+CP Ib	RMP	RMP CP+Ia	RMP CP+Ib
6s - 6p	1/2-1/2	1.86 E8	1.46 E8	1.28 E8	1.	1.	1.
	1/2-3/2	2.57 E8	2.06 E8	1.83 E8	1.952	1.994	2.019
6s - 7p	1/2-1/2	5.90 E5	2.04 E6	6.48 E6	1.	1.	1.
	1/2-3/2	1.12 E7	1.31 E6	4.30 E2	35.96	1.221	0.0005
6s - 8p	1/2-1/2	4.96 E4	4.29 E6	8.91 E6	1.	1.	1.
	1/2-3/2	2.54 E6	7.28 E4	1.42 E6	100.2	0.033	0.313
6s - 9p	1/2-1/2	1.43 E5	3.43 E6	6.69 E6	1.	1.	1.
	1/2-3/2	9.56 E5	2.67 E5	1.59 E6	13.27	0.154	0.472
6s - 10p	12/-1/2	1.44 E5	2.47 E6	4.70 E6	1.	1.	1.
	1/2-3/2	4.64 E5	2.84 E5	1.30 E6	6.419	0.229	0.551
6s - 11p	1/2-1/2	1.20 E5	1.77 E6	3.33 E6	1.	1.	1.
	1/2-3/2	2.61 E5	2.44 E5	1.00 E6	4.346	0.275	0.598
6s - 12p	1/2-1/2	9.42 E4	1.28 E6	2.39 E6	1.	1.	1.
	1/2-3/2	1.61 E5	1.96 E5	7.54 E5	3.412	0.306	0.630
6s - 13p	1/2-1/2	7.26 E4	9.35 E5	1.74 E6	1.	1.	1.
	1/2-3/2	1.06 E5	1.53 E5	5.68 E5	2.907	0.327	0.651
6p - 7s	1/2-1/2	9.06 E7	9.45 E7	9.68 E7	1.	1.	1.
	3/2-1/2	1.76 E8	1.73 E8	1.74 E8	2.774	2.698	2.661
6p - 8s	1/2-1/2	3.50 E7	3.68 E7	3.82 E7	1.	1.	1.
	3/2-1/2	6.46 E7	6.35 E7	6.45 E7	2.279	2.161	2.111
6p - 9s	1/2-1/2	1.78 E7	1.87 E7	1.95 E7	1.	1.	1.
	3/2-1/2	3.27 E7	3.21 E7	3.24 E7	2.196	2.072	2.006
6p - 10s	1/2-1/2	1.03 E7	1.09 E7	1.14 E7	1.	1.	1.
	3/2-1/2	1.90 E7	1.87 E7	1.89 E7	2.167	2.034	1.964
6p - 11s	1/2-1/2	6.34 E6	6.92 E6	7.24 E6	1.	1.	1.
	3/2-1/2	1.16 E7	1.18 E7	1.19 E7	2.152	2.012	1.941
6p - 12s	1/2-1/2	4.25 E6	4.64 E6	4.86 E6	1.	1.	1.
	3/2-1/2	7.76 E6	7.92 E6	8.00 E6	2.143	1.998	1.927
6p - 13s	1/2-1/2	2.95 E6	3.23 E6	3.39 E6	1.	1.	1.
	3/2-1/2	5.40 E6	5.50 E6	5.56 E6	2.137	1.988	1.917
6p - 14s	1/2-1/2	2.10 E6	2.30 E6	2.41 E6	1.	1.	1.
	3/2-1/2	3.84 E6	3.91 E6	3.95 E6	2.133	1.982	1.911
6p - 6d	1/2-3/2	2.81 E8	2.69 E8	2.63 E8	3.830	3.888	3.918
	3/2-3/2	5.47 E7	5.14 E7	4.99 E7	1.	1.	1.
	3/2-5/2	3.21 E8	3.04 E8	2.96 E8	8.494	8.538	8.560
6p - 7d	1/2-3/2	1.14 E8	1.02 E8	9.64 E7	4.542	4.689	4.762
	3/2-3/2	2.05 E7	1.77 E7	1.64 E7	1.	1.	1.
	3/2-5/2	1.24 E8	1.09 E8	1.02 E8	8.977	9.086	9.148
6p - 8d	1/2-3/2	5.84 E7	5.01 E7	4.61 E7	4.817	5.002	5.120
	3/2-3/2	1.01 E7	8.36 E6	7.51 E6	1.	1.	1.
	3/2-5/2	6.24 E7	5.23 E7	4.75 E7	9.149	9.291	9.380
6p - 9d	1/2-3/2	3.41 E7	2.85 E7	2.59 E7	4.957	5.172	5.316
	3/2-3/2	5.82 E6	4.66 E6	4.11 E6	1.	1.	1.
	3/2-5/2	3.61 E7	2.95 E7	2.63 E7	9.240	9.402	9.503

Table 4. (*Contd*).

Transition	J - J	Transition Probabilities			Relative line strengths		
		RMP	RMP+CP Ia	RMP+CP Ib	RMP	RMP CP^+Ia	RMP CP^+Ib
6p - 10d	1/2-3/2	2.17 E7	1.79 E7	1.60 E7	5.040	5.278	5.439
	3/2-3/2	3.66 E6	2.88 E6	2.51 E6	1.	1.	1.
	3/2-5/2	2.28 E7	1.83 E7	1.61 E7	9.343	9.472	9.594
6p - 11d	1/2-3/2	1.46 E7	1.19 E7	1.06 E7	5.132	5.350	5.522
	3/2-3/2	2.45 E6	1.90 E6	1.64 E6	1.	1.	1.
	3/2-5/2	1.53 E7	1.21 E7	1.06 E7	9.392	9.532	9.658
6p - 12d	1/2-3/2	1.02 E7	8.21 E6	7.28 E6	5.132	5.400	5.580
	3/2-3/2	1.70 E6	1.30 E6	1.12 E6	1.	1.	1.
	3/2-5/2	1.07 E7	8.38 E6	7.29 E6	9.392	9.590	9.725
6p - 13d	1/2-3/2	7.24 E6	5.81 E6	5.14 E6	5.159	5.437	5.623
	3/2-3/2	1.21 E6	9.18 E5	7.84 E5	1.	1.	1.
	3/2-5/2	7.64 E6	5.94 E6	5.15 E6	9.452	9.656	9.799
5d - 5f	3/2-5/2	2.94 E8	2.55 E8	2.40 E8	12.62	12.59	12.64
	5/2-5/2	2.14 E7	1.85 E7	1.74 E7	1.	1.	1.
	5/2-7/2	3.06 E8	2.67 E8	2.53 E8	18.99	19.16	19.29
5d - 6f	3/2-5/2	1.80 E8	1.51 E8	1.39 E8	12.99	13.00	12.92
	5/2-5/2	1.29 E7	1.08 E7	1.00 E7	1.	1.	1.
	5/2-7/2	1.87 E8	1.59 E8	1.49 E8	19.32	19.60	19.75
5d - 7f	3/2-5/2	1.10 E8	8.99 E7	8.17 E7	13.16	13.18	13.11
	5/2-5/2	7.84 E6	6.39 E6	5.83 E6	1.	1.	1.
	5/2-7/2	1.14 E8	9.45 E7	8.69 E7	19.44	19.71	19.85
5d - 8f	3/2-5/2	7.11 E7	5.70 E7	5.13 E7	13.25	13.27	13.23
	5/2-5/2	5.04 E6	4.04 E6	3.64 E6	1.	1.	1.
	5/2-7/2	7.38 E7	5.98 E7	5.43 E7	19.51	19.76	19.90
5d - 9f	3/2-5/2	4.81 E7	3.81 E7	3.41 E7	13.31	13.32	13.30
	5/2-5/2	3.40 E6	2.69 E6	2.41 E6	1.	1.	1.
	5/2-7/2	5.00 E7	4.00 E7	3.60 E7	19.57	19.82	19.95
7s - 7p	1/2-1/2	2.57 E7	2.53 E7	2.51 E7	1.	1.	1.
	1/2-3/2	3.54 E7	3.48 E7	3.45 E7	1.903	1.909	1.912
7s - 8p	1/2-1/2	4.50 E5	2.37 E5	1.48 E5	1.	1.	1.
	1/2-3/2	2.84 E6	2.29 E6	1.99 E6	11.76	18.00	25.18
7p - 8s	1/2-1/2	2.00 E7	2.03 E7	2.05 E7	1.	1.	1.
	3/2-1/2	3.66 E7	3.70 E7	3.72 E7	2.623	2.607	2.594
7p - 9s	1/2-1/2	8.24 E6	8.71 E6	8.70 E6	1.	1.	1.
	3/2-1/2	1.42 E7	1.45 E7	1.47 E7	2.074	2.007	2.033
7p - 7d	1/2-3/2	4.15 E7	4.20 E7	4.23 E7	3.708	3.735	3.758
	3/2-3/2	8.62 E6	8.66 E6	8.67 E6	1.	1.	1.
	3/2-5/2	5.04 E7	5.07 E7	5.08 E7	8.390	8.407	8.413
7p - 8d	1/2-3/2	2.14 E7	2.17 E7	2.13 E7	4.416	4.547	4.503
	3/2-3/2	4.10 E6	4.04 E6	4.00 E6	1.	1.	1.
	3/2-5/2	2.46 E7	2.44 E7	2.42 E7	8.850	8.886	8.906
6d - 6f	3/2-5/2	5.44 E6	5.27 E6	5.40 E6	10.48	10.56	10.66
	5/2-5/2	4.89 E5	4.70 E5	4.77 E5	1.	1.	1.
	5/2-7/2	6.75 E6	6.64 E6	6.81 E6	18.32	18.77	18.95
6d - 7f	3/2-5/2	7.78 E6	7.63 E6	7.80 E6	11.78	11.53	11.36
	5/2-5/2	6.31 E5	6.32 E5	6.56 E5	1.	1.	1.
	5/2-7/2	9.02 E6	9.22 E6	9.62 E6	19.02	19.40	19.55

(c) *Transition probabilities and relative line strengths*

A much stronger influence of core polarization may be seen for transition probabilities or oscillator strengths (Table 4). Oscillator strengths are not listed in this paper but the data can be obtained from the author or deduced from transition probabilities. Unfortunately, higher transitions of principal series are strongly affected by mutual cancellation (up to 98%) of the positive and negative contributions in the radial transition integral. This is also the case for the dramatic deviation in the relative line strengths from the statistical ratio of 1 : 2 (see Table 4). In the cancellation region, the radial integral is extremely sensitive to changes in wavefunctions and, therefore, the influences of core polarization and spin-orbit interaction (which is responsible for the deviation of relative line strengths from the statistical values) on transition probabilities are greatly enhanced. For transitions with $\Delta n = 0$, which are not strongly affected by cancellation (the cancellation is only 0.2 and 0.8% for $n = 6$ and $n = 7$, respectively), core polarization reduces the transition probabilities and oscillator strengths. This effect is particularly apparent for $6s$–$6p$ transition where the reduction amounts to about 30%.

Measured oscillator strengths are only available for the $6s\ ^2S_{1/2} - 6p\ ^2P_{1/2,\,3/2}$ transitions. They are 0.29 ± 0.02,[4] 0.275 ± 0.03[3] and 0.30 ± 0.03,[2]† for the $6s\ 2S_{1/2} - 6p\ ^2P_{1/2}$ transition and 0.58 ± 0.03,[4] 0.55 ± 0.06[3] and 0.45 ± 0.05[2] for the $6s\ ^2S_{1/2} - 6p\ ^2P_{3/2}$ transition. These data may be compared with the results of the present study for RMP + CP Ib, which yields 0.262 and 0.594 for the two components of the doublet and with the values obtained previously by the author[5] from the relativistic Hartree–Fock method with core polarization (0.262 and 0.597). In both cases, $\alpha_c = 11.14\ a_0^3$ was used. The data obtained with core polarizability suggested by Fraga *et al.*[9] ($7.36\ a_0^3$) show considerably larger disagreement with experiments. Reductions due to core polarization occur also for most of the transitions in the diffuse (np–md) and fundamental (nd–mf) series, whereas for the sharp ($np - (n+1)s$) series a small increase is found in the transition probabilities.

(d) *Static dipole polarizability of* Yb^+

The computed oscillator strengths for singly-ionized ytterbium permit computation of the static dipole polarizability for this system. Employing the well-known relation[11]

$$\alpha_d = 4R^2 \sum_{n=n_0}^{\infty} f_{n_0 - n} \lambda^2_{n_0 - n}, \tag{5}$$

where R is Rydberg's constant ($R = 109737.3\ \mathrm{cm}^{-1}$), while f_{n_0-n} and λ_{n_0-n} are respectively, absorption oscillator strengths and calculated wavelengths (in cm^{-1}) for the $n_0 s - np$ transitions with $n_0 = 6$, we obtain different values of α_d for different types of calculations. If oscillator strengths not corrected for polarization of the Yb^{2+}-like core are used (RMP), $68.47\ a_0^3$ is obtained, whereas the core-polarization-corrected oscillator strengths yield $54.48\ a_0^3$ (RMP + CP Ia) and $48.18\ a_0^3$ (RMP + CP Ib). Employing the Hartree–Fock method without inclusion of the valence-core electron correlation, Fraga *et al.*[9] obtained the dipole polarizability $67.3\ a_0^3$ for Yb^+. Because of cancellation effects, almost all of the contributions to the sum in Eq. (5) arise from the $6s$–$6p$ transition (99.8, 99.9, and 99.8% for RMP, RMP + CP Ia and Ib, respectively). In view of the dominant contribution made by this transition to the dipole polarizability of Yb^+, we have tried to evaluate a lower bound for this quantity by employing the measured oscillator strengths. The resulting values are 42.1 ± 4.5, 46.4 ± 5.1 and $48.9 \pm 2.8\ a_0^3$ for the data reported by Andersen *et al.*,[2] Penkin *et al.*,[4] and Rambow and Schearer,[3] respectively. The theoretical value closest to the estimated lower bound is $48.18\ a_0^3$, which was obtained by including core polarization and using the polarizability of the Yb^{2+} – like core of $11.14\ a_0^3$.

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