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Transition probabilities of forbidden lines in Pb I

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Abstract. Multiconfiguration Dirac-Fock as well as semiempirical calculations of decay rates of forbidden transitions within the ground $6s^26p^2$ configuration of neutral lead are reported and compared with relativistic Hartree-Fock results as well as with available experimental data.

PACS. 31.10+z Theory of electronic structure, electronic transitions, and chemical binding – 31.15.Ar Ab initio calculations – 31.15.Ct Semi-empirical and empirical calculations (differential overlap, Hückel, PPP methods, etc.)

1 Introduction

Decay rates calculated for strong transitions are in reasonable agreement with experiment, but in the case of weak transitions the predictions often strongly disagree with the experimental data. It results from the fact that weak transition rates are especially sensitive to even small modifications to the wave functions and a careful choice of the theoretical method to be used is required.

The $6s^26p^2$ ground configuration of lead gives rise to the five levels $^1D_2$, $^3P_{2,1,0}$ and $^1S_0$. Since electric-dipole transitions between states of the same parity are forbidden, all the $6s^26p^2$ excited levels are metastable. Weak magnetic-dipole ($M1$) and electric-quadrupole ($E2$) transitions between these levels are permitted in the second-order radiation theory.

A complete list of $M1$ and $E2$ transition probabilities within the $6p^2$ configuration of Pb I has been published by Garstang [1]. However, the calculated rates strongly disagree with experiments [2,3] mainly because of very rough estimate of the adopted s_q value. Calculations presented in [4] better agree with experiment.

Recently, several papers using multiconfigurational methods have been published. Two of them, by Dzuba *et al.* [5] and Chou *et al.* [6] dealt with the $^3P_1$-$^3P_0$ $M1$ transition rate, which is of great importance in the investigation of parity-nonconserving effects in atoms. Dzuba *et al.* [5] used the relativistic Hartree-Fock (HFR) method improved upon by including polarisation and correlation corrections. Chou *et al.* [6] obtained the result by using the multiconfiguration relativistic random-phase approximation (MCRRPA) method.

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Table 1. Comparison between experimental and theoretical results for $E2$ contributions in mixed ($M1+E2$) transitions in Bi I.

Transition	λ(nm)	$E2$ admixture (%)		
		Experiment	HFR theory[d]	Semiempirical values[e]
$^2P_{3/2}$-$^2D_{5/2}$	564.0	28 ± 3[a]	34	24
$^2P_{3/2}$-$^2D_{3/2}$	459.7	2.5 ± 0.5[b]	3.3	2.7
$^2P_{1/2}$-$^4S_{3/2}$	461.5	6.5 ± 0.5[b]	23	7.3
$^2D_{5/2}$-$^4S_{3/2}$	647.6	16 ± 1[b] 17 ± 1[c]	35	17
$^2D_{3/2}$-$^4S_{3/2}$	875.5	2.25 ± 0.5[a, f] 1 ± 1[c]	1.3	0.5

[a] [24].
[b] [25].
[c] [10].
[d] [7].
[e] The results were obtained by using the intermediate-coupling wave functions from [9] and the experimental value of the radial integral $s_q = 8.7\ ea_0^2$ from [10].
[f] The result for 875.5 nm transition is probably too high and can be deformed by systematic error [26].

The most extensive multiconfiguration calculations of multipole transition rates for states within the $6p^k$ ($k = 1, \ldots, 5$) configurations in the thallium, lead, bismuth, polonium and actinium sequences up to radon have been performed by Biémont and Quinet [7] using the HFR method. In the HFR method the transition rates are computed in intermediate coupling with basis functions obtained in the framework of the Slater-Condon theory, where electrostatic and spin-orbit integrals are evaluated so as to fit the observed energy levels. The HFR

energies obtained in [7] appear in very good agreement with experimental energy levels, but the agreement with experimental data concerning multipole transition rates for neutral atoms is not that satisfactory. For instance in the case of transition rates for the ground configuration of Bi I the experimental transition probability $A(^2D_{3/2}$-$^4S_{3/2}) = 22.5 \pm 1.4$ s^{-1} [8] is almost 50% lower than the theoretical result. Furthermore, there is also a large discrepancy between measured and calculated admixtures of $E2$ radiation in mixed transitions (see Tab. 1). As follows from the table much better agreement (except for the $^2D_{3/2}$-$^4S_{3/2}$ transition) can be achieved in semiempirical single-configuration calculation, where we used the Landman and Lurio [9] intermediate-coupling wave functions and experimental value of the radial integral s_q of r^2 between single-electrons states, $s_q = 8.7ea_0^2$ from [10]. In the case of Pb I the lack of experimental data has not allowed us to verify the HFR results directly. The most precisely determined experimental result concerning the forbidden transitions within the $6s6p^2$ configuration of Pb I is the ratio of intensities of the 461.9 nm and 531.5 nm lines. The experimental value 5.06 ± 0.25 [2] is larger than the HFR result $I_{461.9}/I_{531.5} = 3.26$.

The HFR method allows to consider a large number of interacting configurations, but only approximately accounts for the relativistic effects, which are crucial for heavy elements. In the recent years, the multiconfiguration Dirac-Fock (MCDF) method has played an important role in calculations of atomic structure and transition rates for various atomic systems. The MCDF method is an *ab initio* and fully relativistic method and is expected to provide accurate results for heavy atoms and ions. On the other hand, the convergence problems in MCDF calculations strongly limit the consideration of electron-correlation effects.

In this paper we apply the MCDF method to the forbidden transitions in Pb I. For comparison we also performed semiempirical single-configuration calculations concerning cumulative correlation effects of perturbing configurations represented by appropriate effective parameters. The results obtained are compared with HFR results as well as with available experimental data.

2 MCDF calculations

In the calculations the unpublished numerical code GRASP^2 [11] has been used. This is the newest version of the GRASP code described by Dyall *et al.* [12]. A new element in GRASP^2 is a radial part of the program, now based on the algorithm introduced by Sienkiewicz and Baylis [13]. It accelerated the convergence of the self-consistent field (SCF) process.

The MCDF method is based on a fully relativistic Dirac-Coulomb Hamiltonian:

$$\widehat{H}^{\mathrm{DC}} = \sum_i \hat{h}_i + \sum_{i<j} \frac{1}{|\hat{\mathbf{r}}_i - \hat{\mathbf{r}}_j|}, \qquad i,j = 1,\ldots,N\,. \quad (1)$$

Here $\hat{h}_i$ is a single-electron Dirac Hamiltonian which can be written as

$$\hat{h}_i = c\sum_{k=1}^{3} \alpha_k^i \hat{p}_k^i + (\beta^i - 1)c^2 + V_{\mathrm{nuc}}(\hat{\mathbf{r}}_i)\,, \quad (2)$$

where α^i and β^i are usual Dirac matrices, c is the velocity of light and V_{nuc} is the potential of the nucleus.

In the MCDF formulae the atomic state function is given by a multiconfiguration wave function of the form

$$|\, \Gamma PJM\rangle = \sum_{r=1}^{n_c} c_{r\Gamma}\, |\, \gamma_r PJM\rangle\,, \quad (3)$$

where P is the parity of the atomic state, J the total angular momentum, M the magnetic number, and $c_{r\Gamma}$ are configuration mixing coefficients. Each $|\, \gamma_r PJM\rangle$ is an eigenstate of total angular momentum and parity operators, constructed as a Slater determinant from relativistic one-electron orbitals. The label γ_r represents all information (occupation of different subshells, coupling schemes, seniority numbers) required to define the configuration state function uniquely. In the MCDF method the radial parts of functions $|\, \gamma_r PJM\rangle$ as well as the mixing coefficients $c_{r\Gamma}$ are generated in the SCF process.

The MCDF calculations have been performed with various basis sets. The choice of these sets was based on studies of other authors. Flambaum *et al.* [14] and Biémont and Hansen [15] found that the admixture of the highly excited $6p^4$ configuration to the ground $6s^26p^2$ configuration is the most important. The multiconfiguration calculations are hampered by severe convergence problems in the SCF process, which increase with the number of configurations included. We present the results of calculations for the following basis sets:

MCDF (1) $6s^26p^2$,
MCDF (2) $6s^26p^2 + 6p^4$,
MCDF (3) $6s^26p^2 + 6p^4 + 6s^26p7p$,
MCDF (4) $6s^26p^2 + 6s^26p5f$.

There are several types of calculations, regarding the choice of the energy functional, available with the code used here. They are described in detail by Grant [16]. All our calculations have been performed in the average level (AL) scheme, in which the energy functional is averaged over a set of states with the same total angular momentum J and the same parity. The spin-orbitals used are common for all the configurations involved in the calculations. The choice of the AL option was suggested by calculations performed by Rose *et al.* [17] for Bi I and by Bieroń *et al.* [18] for Pb I, where the best results were obtained for the AL version.

In the present calculation higher order relativistic corrections have been included. Among them the dominant contribution comes from the Breit interaction yielding a dynamic correction to the static Coulomb interaction. Furthermore, the effect of a finite nuclear size has been included. The Fermi statistical model has been

Table 2. Transition probabilites for the ground $6s^26p^2$ configuration of Pb I (in s^{-1}) in the MCDF approximation calculated with theoretical (T) and experimental (E) values of the transition energies.

Transition	λ(nm)	MCDF(1) $(6s^26p^2)$				MCDF(2) $(6s^26p^2+6p^4)$				MCDF(3) $(6s^26p^2+6p^4+6s^26p7p)$				MCDF(4) $(6s^26p^2+6s^26p5f)$	
		A^{M1}		A^{E2}		A^{M1}		A^{E2}		A^{M1}		A^{E2}		A^{M1}	A^{E2}
		(T)	(E)	(T)	(E)	(T)	(E)	(T)	(E)	(T)	(E)	(T)	(E)	(T)	(T)
$^1S_0 \rightarrow {}^1D_2$	1248.6	0	0	0.03^V	0.01^V	0	0	0.02^V	0.02^V	0	0	0.008^V	0.01^V	0	0.06^V
				0.19^L	0.04^L			0.06^L	0.05^L			0.15^L	0.15^L		0.31^L
$^3P_2$	531.5	0	0	2.43^V	1.08^V	0	0	1.79^V	1.81^V	0	0	3.10^V	3.60^V	0	2.43^V
				59.51^L	26.33^L			21.06^L	21.27^L			24.41^L	28.35^L		55.52^L
$^3P_1$	461.9	97.97	57.05	0	0	73.07	65.16	0	0	66.78	64.42	0	0	99.61	0
$^1D_2 \rightarrow {}^3P_2$	925.3	12.83	11.27	0.77^V	0.62^V	9.36	10.49	0.66^V	0.80^V	9.06	10.49	0.61^V	0.78^V	11.69	0.74^V
				0.95^L	0.76^L			0.51^L	0.62^L			0.57^L	0.73^L		0.62^L
$^3P_1$	733.2	15.29	11.36	0.71^V	0.43^V	10.91	9.84	0.61^V	0.51^V	10.52	9.85	0.48^V	0.43^V	13.63	0.68^V
				0.74^L	0.45^L			0.38^L	0.32^L			0.33^L	0.30^L		0.49^L
$^3P_0$	466.0	0	0	0.43^V	0.40^V	0	0	0.51^V	0.63^V	0	0	0.42^V	0.53^V	0	0.52^V
				0.80^L	0.74^L			0.71^L	0.87^L			1.10^L	1.38^L		0.65^L
$^3P_2 \rightarrow {}^3P_1$	3532.2	0.47	0.20	$12.5(-4)^{V\,a}$	$3.0(-4)^V$	0.47	0.21	$16.9(-4)^V$	$4.4(-4)^V$	0.45	0.21	$16.1(-4)^V$	$4.5(-4)^V$	0.57	$18.3(-4)^V$
				$18.9(-4)^L$	$4.5(-4)^L$			$15.7(-4)^L$	$4.1(-4)^L$			$15.6(-4)^L$	$4.4(-4)^L$		$17.4(-4)^L$
$^3P_0$	938.9	0	0	0.43^V	0.45^V	0	0	0.41^V	0.51^V	0	0	0.34^V	0.42^V	0	0.39^V
				0.19^L	0.20^L			0.14^L	0.17^L			0.18^L	0.22^L		0.11^L
$^3P_1 \rightarrow {}^3P_0$	1278.9	4.78	7.38	0	0	4.11	7.24	0	0	4.29	7.27	0	0	4.05	0

[a] The number in parenthesis denotes power of 10, *i.e.* $12.5(-4)$ denotes 12.5×10^{-4}.

Table 3. Observed and calculated energy levels of the ground configuration of Pb I.

Energy level	Experiment	Calculated energies			
		MCDF (1)	MCDF (2)	MCDF (3)	MCDF (4)
$^3P_0$	0	0	0	0	0
$^3P_1$	7819.35	6763.94	6474.75	6558.51	6357.46
$^3P_2$	10650.47	10538.19	10186.31	10205.90	10304.39
$^1D_2$	21457.90	21824.18	20590.42	20498.79	21476.56
$^1S_0$	29466.81	32686.72	28964.42	28467.70	33576.76
$\sqrt{\sum_i (E_i - E_i^{\rm exp})^2}$		3410	1740	1925	4376

used with the root-mean-squared radius of the nucleus $r_{\rm rms} = 0.836\ A^{1/3} + 0.570$ fm [19], where A is the atomic mass number.

The calculated *ab initio* transition probabilities are presented in Table 2. The $E2$ transition rates were computed using fully relativistic forms of the transition operators in both the Babushkin and the Coulomb gauges (respectively, the "length" (L) and the "velocity" (V) formalisms in non-relativistic approximation). Discrepancies between these two gauges are a consequence of the finite basis approximation together with the SCF approach (see [20] for details). The choice of the gauge is a very difficult problem. In many cases better results were obtained using the "length" form. In contrast, Grant [20] has estimated that the"velocity" gauge, which plays a privileged role for the MCDF variational calculations, should be preferred. Besides, some other authors recommend values of transition rates lying between the L and the V gauges. Then, comparison with experimental values is always required.

The computed energies of states under consideration are presented in Table 3. For the energy levels we used the data given by Moore [21]. At the bottom of the table the total sum of departures from the experimental values for each version of the calculation employed is presented. It provides some information about the level of accuracy of the calculated transition rates. In the case of MCDF(2) and MCDF(3) the agreement between the calculated and experimental energies is satisfactory. With the exception of the $^3P_1$, for each of the energy levels the departures from the experimental values are in the range of $3 \div 4\%$ (for the $^3P_1$ level the departure is about 17%). Table 3 shows that the inclusion in the calculation of the most strongly interacting configuration $6p^4$ significantly improves the agreement with the observed energy levels in comparison with the MCDF(1) version and that mixings with the excited $6s^2 6p7p$ and $6s^2 6p5f$ configurations are of minor importance.

From Table 2 it follows that also for calculated transition rates the mixing between the $6s^2 6p^2$ and $6p^4$ configurations plays an important role. The inclusion in the calculation of the $6s^2 6p7p$ configuration in the MCDF (3) version causes only small changes. However, they are more significant for $E2$ than for $M1$ rates. The $6p^4$ configuration proved to have the largest contribution among all the admixed configurations, but the mixing rate is not as high as one might have expected. The contribution from all interacting levels of the $6p^4$ configuration to the ground $6s^2 6p^2\ ^3P_0$ state was found to be 0.8%. Mixings between $6s^2 6p^2$ and other excited configurations involving $5f$ electrons are much weaker. As an example we present result in the version MCDF (4).

Table 4. $E2$-transition probabilites (in s^{-1}) calculated by using the MCDF and CI methods.

Transition	λ(nm)	$E2$-transition rates	
		CI	MCDF(3)
$^1S_0$-$^1D_2$	1248.6	0.08^V	0.008^V
		0.14^L	0.15^L
$^1S_0$-$^3P_2$	531.5	2.40^V	3.10^V
		25.50^L	24.41^L
$^1D_2$-$^3P_0$	466.0	0.39^V	0.42^V
		1.05^L	1.10^L
$^3P_2$-$^3P_0$	938.9	0.29^V	0.34^V
		0.19^L	0.18^L

The changes caused by the inclusion in the MCDF calculations of the successive configurations are more evident in transition rates calculated with experimental values of the transition energies. Here, differences between values obtained in sequential versions of calculations are only effected by modifications of the transition amplitude in the matrix element. Since the energy of the $^3P_1$ level was not well approximated in our calculations, the differences between several rates presented in (T) columns of Table 2 in comparison with their counterparts in (E) columns are significant.

3 CI calculations

The effect of the $6s$, $6p \rightarrow 6d$ excitations was analysed separately in the relativistic configuration interaction (CI) approach. Two-step calculations were carried out. Firstly, the single spin-orbitals were calculated by means of the self-consistent-field method. Next, these atomic orbitals were used to construct multiconfigurational $6s^2 6p^2 + 6p^4 + 6s^2 6p7p + 6s6p^2 6d + 6s^2 6d^2 + 6p^2 6d^2 + 6s^2 7p^2 + 6p^2 7p^2$ state functions by performing the configuration-interaction calculations. As in the case of HFR calculations [7] the choice

Table 5. Calculated semiempirical transition probabilities for the ground $6s6p^2$ configuration of Pb I (in s^{-1}).

		$M1$-transitions		$E2$-transitions	
Transition	λ(nm)	Semi-empirical	HFR[a]	Semi-empirical	HFR[a]
$^1S_0$-$^1D_2$	1248.6	0	0	0.56	0.42
$^3P_2$	531.5	0	0	17.33	18.66
$^3P_1$	461.9	70.10	52.91	0	0
$^1D_2$-$^3P_2$	925.3	12.76	10.58	0.78	0.95
$^3P_1$	733.2	16.65	14.45	0.69	0.73
$^3P_0$	466.0	0	0	0.12	0.17
$^3P_2$-$^3P_1$	3532.2	0.16	0.40	2.8×10^{-4}	1.3×10^{-3}
$^3P_0$	938.9	0	0	0.25	0.49
$^3P_1$-$^3P_0$	1278.9	7.50	7.85	0	0

[a] [7].

Table 6. Comparison between observed and calculated intensity ratios of multipole lines in Pb I.

	$I_{461.9}/I_{531.5}$	$I_{466.0}/I_{733.2}$	$I_{925.3}/I_{733.2}$
Experiment	5[a]	0.023[a]	0.84[a]
	5.06 ± 0.25[b]		
Theory			
MCDF (1)	$3.64^{(T)}$	$0.061^{(T)}$	$0.68^{(T)}$
	$4.79^{(E)}$	$0.076^{(E)}$	$0.80^{(E)}$
MCDF (2)	$7.36^{(T)}$	$0.084^{(T)}$	$0.69^{(T)}$
	$6.50^{(E)}$	$0.115^{(E)}$	$0.87^{(E)}$
MCDF (3)	$5.58^{(T)}$	$0.109^{(T)}$	$0.70^{(T)}$
	$4.64^{(E)}$	$0.147^{(E)}$	$0.87^{(E)}$
Semiempirical	4.65	0.011	0.62
HFR	3.26	0.018	0.60

Letters in parentheses label ratios for transition rates calculated with theoretical (T) and experimental (E) energies.
[a] [3].
[b] [2].

of configurations for the basis set was based on the Layzer complex concept. Results of such an analysis for $E2$ transitions with $\Delta J = 2$ are presented in Table 4. For these transitions a large difference appears between the Babushkin and the Coulomb gauges in the MCDF calculations. However, using the CI approach with a larger number of configurations the disagreement between these two formalisms was not reduced. Moreover, it caused only small changes of the calculated rates (considering the discrepancy between different gauges) in comparison with the MCDF(3) results. The exception makes only the value of the $^1S_0$-$^1D_2$ rate in the "velocity" formalism, which is 10 times larger in the CI calculation. It seems that the correlation effects, which could improve the agreement between different gauges, arise from mixing between $6p^2$ and a very large number of weakly interacting configurations.

4 Semiempirical transition probabilities in single-configuration approximation

The results of the MCDF calculations show that the ground configuration of Pb I may be regarded as a pure configuration. All the states of this configuration were found to be pure with percentage contribution of the leading configuration exceeding 98%. This conclusion follows also from the analysis of sums of the g_J factors for $J = 1$ and $J = 2$. Therefore, for comparison with the HFR and MCDF results we performed semiempirical calculations in the single-configuration approximation. The results obtained for the similar case of Bi I and presented in Table 1 show that calculations performed by using the fitting procedure in the single-configuration approximation give more reliable transition rates than multiconfigurational calculations.

In the calculation presented here, the effective electrostatic spin-orbit interaction represented by the $Q^{(2)}$ parameter introduced by Goldschmidt *et al.* [22] was included. The $Q^{(2)}$ parameter allows to consider a significant part of the magnetic interaction, provided by the Breit equation, and which was neglected in earlier calculations [4]. A least-squares fit to the experimental energy levels treating the Slater integrals, spin-orbit constant, α and $Q^{(2)}$ as adjustable parameters yielded the following values: $F_0 = 16806.1$ cm^{-1}, $F_2 = 888.6$ cm^{-1}, $\xi_p = 7714.4$ cm^{-1}, $\alpha = -249.3$ cm^{-1} and $Q^{(2)} = 2253.5$ cm^{-1}. The calculated energy levels agree exactly with observation as a consequence of the fact that the number of energy levels is equal to the number of free parameters. The value of the radial integral $s_q = e\int_0^\infty P_{6p} r^2 P_{6p} \mathrm{d}r$ needed for computation of the $E2$ transition rates was deduced from the observed $M1$-$E2$ interference effect on the 733.2 nm line [23]. This yielded $s_q = 12.24 \pm 1.59\, ea_0^2$. So determined the s_q value is independent of the choice of the intermediate coupling coefficients. Results of calculations are shown in Table 5 together with the HFR results.

5 Discussion of the results

The $M1$ transition probabilities calculated with experimental values of the transition energies in the MCDF(3) version agree with the HFR results within 20–30%, although in the case of the weakest $^3P_2$-$^3P_1$ transition the difference reaches 50%. Larger discrepancy appears for the $E2$ components. If we use, for A^{E2} rates, the mean values between both the L and the V gauges, the differences between MCDF(3) and HFR results reach 80%, although again, the largest discrepancy appears for the $^3P_2$-$^3P_1$ transition, which is an order of magnitude lower than the HFR result.

For most of the $E2$ rates the agreement between semiempirical and HFR results is very good, particularly if we take into account the error bar connected with the s_q value. The largest difference appears only for the weakest $^3P_2$-$^3P_1$ transition, which is an order of magnitude lower than the HFR result. For $M1$ rates the differences

between semiempirical and HFR results are more significant. For most of the transitions the agreement is within 20%. However, again in the case of $^3P_2$-$^3P_1$ the difference reaches 40% and in the case of $^1S_0$-$^3P_1$ (461.9 nm) the semiempirical $M1$ rate is 25% bigger.

The $M1$ $^3P_1$-$^3P_0$ transition rate interesting for the parity-violating experiment was also calculated by Dzuba *et al.* [5] and Chou *et al.* [6]. The $M1$ transition amplitude calculated by Dzuba *et al.* [5] equals $-0.741\ \mu_B$. It corresponds to $A^{M1} = 7.08\ s^{-1}$ and $f = 5.208 \times 10^{-7}$ au which are in disagreement with the A^{M1} and f values quoted by Chou *et al.* [6] and Biémont and Quinet [7]. The oscillator strength obtained by Chou *et al.* [6], $f = 5.152 \times 10^{-7}$ au, corresponds to $A^{M1} = 7.00\ s^{-1}$.

Calculated transition probabilities can be tested by comparison with experimental intensity ratios. This is done in Table 6 (for A^{E2} rates, in calculated intensity ratios we used mean values between both the V and the L gauges). The most important test is a comparison between calculated and experimental values for $I_{461.9}/I_{531.5}$. The ratio obtained in the MCDF(1) and MCDF(3) versions agree better with the observed value than the HFR result. It is caused by a 20% larger $M1$ rate (461.9 nm) obtained in the MCDF calculations.

Moreover, a 4.8% admixture of $E2$ radiation in the mixed 733.2 nm transition, obtained in HFR calculations, seems to be slightly too high, although the value is in the upper limit of the experimental result $4 \pm 1\%$ [23]. In MCDF calculations, for the transition $^1D_2$-$^3P_1$ (733.2 nm), the calculated contribution of $E2$ radiation is in the range between 3.6%, for MCDF(3), and 4.7% for MCDF (1), in good agreement with the experimental value.

6 Conclusions

The results show that even a very limited effect of configuration mixing considered in the calculation significantly improves the agreement of calculated transition energies with experiment. The situation is more complex in the case of transition probabilities. The influence of admixed configurations is very weak and their limited inclusion in the calculations does not necessarily improve the agreement with experiment, even if the calculated energy levels better agree with observation.

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