

# Electron affinity and hyperfine structure constants of $Pa^-$ : $7p$ attachment.

By

Konstantin D. Dinov and Donald R. Beck

Physics Department, Michigan Technological University,

Houghton, MI 49931

Valence shell relativistic configuration interaction calculations for the  $7p$  attachment to the  $Pa$   $I$  ground state yield one bound state, viz.  $Pa^- 5f^26d7s^27p$   $J=6$ , with electron affinity of 0.222 eV. We found no other  $J$ s for this configuration to be bound, nor are any of the  $Pa^- 5f^26d^27s^2$  levels expected to be bound. The hyperfine structure constants for the  $^{231}Pa^-$  bound state are:  $A=741.3$  MHz, and  $B=1309$  MHz. Although the core-valence correlation effects are absent the agreement between the theory ( $4736\text{ cm}^{-1}$ ) and experiment ( $4121\text{ cm}^{-1}$ ) for the position of the first excited state of  $Pa$  is good (15%). We review our previous studies for the  $np$  attachment in Rare Earths to systematically analyze the binding of  $np_{1/2}$  and  $np_{3/2}$  electrons, in these species.

PACS numbers: 32.10Hq, 32.10Fn, 31.30Gs, 31.25Eb

# I. INTRODUCTION

Recently many Rare Earth negative ions were detected, using the accelerator mass spectrometry for both Lanthanides [1–4], and Actinides [3–6]. For most of them, except  $Tm^-$ ,  $Yb^-$  and  $Dy^-$  [1] (which have small electron affinities), only the relative negative ion yields were measured, and there is no experimental information about the Electron Affinity (EA), or characterization (configuration, J) for the negative ion bound states.

To explain those experimental results, a new attachment mechanism of the  $np$  electron was proposed by Vosko *et al.* [7–10], Gribakina *at al.* [11], and ourselves [12–17]. Those studies also found that in addition to the  $np$  attachment, the species with highest yield of negative ions can attach also  $(n - 1)d$  electron, i.e. in  $La^-$  [8],  $Th^-$  [12] and  $Ce^-$  [14,16], or have bound states for several Js, i.e. in  $Th^-$  and  $Ce^-$ . Further, our study of  $Ce^-$  [14,16] found an excited state of the negative ion (J=7/2) bound to the  $Ce I$  ground state.

In this work we report the study of a fourth actinide,  $Pa^-$ , which is found to attach only  $7p$  electron. Previously,  $Ac^-$  [8],  $Th^-$  [12] and  $U^-$  [13] were studied. The Electron Affinity (EA) of 0.222 eV is consistent with the relatively moderate yield for this system [6]. The hyperfine structure result (A=741.3 MHz, B=1309 MHz) for  $^{231}Pa^-$  is the first *ab initio* one for this system. We also analyze the results for  $Pa^-$  and our earlier work on Rare Earth negative ions  $Th^-$  [12],  $U^-$  [13],  $Ce^-$  [14], and  $Pr^-$  [15] to study the pattern in the attachment of  $np_{1/2}$ , and  $np_{3/2}$  electrons.

## II. METHODOLOGY

Our Relativistic Configuration Interaction (RCI) methodology is described in detail in our earlier work [13,14,16,18,19]. We follow those lines, with minor modifications associated with the specifics of the system. The biggest complication in correlating the valence shell electrons of the Rare Earth elements comes from the presence of two or more open  $f$  electrons. Our studies [13,15,16] found an effective mechanism to restrict the  $f$  electron couplings (and thus the number of eigenvectors) by imposing certain J restrictions for this group of electrons.

We begin with Multi-Configurational Dirac-Fock (MCDF) calculations, using the program of Desclaux [20]. The calculations for the neutral and the negative ion provide our zeroth order wavefunction (WF). The electrostatic integrals and the occupation numbers needed in [20] are provided by the structure part of our computer program [21]. For the  $Pa I$  ground state we include the manifolds  $5f^2 [6d7s^2 + 6d^27s + 6d^3 + 6d7p^2 + 7s7p^2]$ , and for  $Pa^-$ ,  $5f^2 [6d7s^27p + 6d^27s7p + 6d^37p + 6d7p^3 + 7s7p^3]$ . This way the system is treated in a balanced way, i.e. the electron correlations in the negative ion are the same as in the neutral, plus the correlation due to the presence of  $7p$  electron. In our study of  $Ur^-$  [13] and  $Pr^-$  [15] the MCDF calculation had convergence problems, which we overcame by iteration. For the negative ion we started with nuclear charge equal to the charge of the neutral + 0.3, and iterated down to the correct value. For  $Pa I$  and  $Pa^-$  the current dimension of the MCDF program (1000 vectors, and 500,000 electrostatic integrals) was enough to include all important MCDF correlations, and we generated the solution for the exact nuclear charge, without iterations. Based on our previous experience [13,16] we used a reduced damping factor, 0.2, for the WF iterations. Still the selfconsistency (SC) was poor, and we repeated the calculations, with the numerical WF from the previous run, to get SC=0.0604 eV for  $Pa^-$  J=6, and SC=0.0892 eV for  $Pa I$ .

In our Relativistic Configuration Interaction (RCI) calculations we use a first order form for the WF by doing single and double excitations from the reference manifolds  $5f^26d7s^2$  for

$Pa I$  and  $5f^2 6d 7s^2 7p$  for  $Pa^-$ . Subshells initially empty are called virtuals, and we represent their radial part by relativistic screened Hydrogenic spinors with screened parameter  $Z^*$  (the angular part is the same as for the MCDF spinors of the same symmetry). The effective charge  $Z^*$  is found by applying the energy minimization principle, during the CI process. The configuration coefficients (parent weights) are found from the corresponding eigenvectors, after the diagonalization of the energy matrix. For  $Pa I$  we had 4854 parents (eigenvectors), and 6840 for  $Pa^-$ , from which only about 300 are energetically and hfs important (energy contribution greater than 0.0001 eV). Based on the spectroscopic labeling [22] we restricted the  $5f^2$  couplings to  $8 \leq 2J \leq 12$ . Because of the compact nature of the  $5f$  orbital (for  $Pa^-$   $\langle r \rangle_{4f} = 1.6a.u.$ ,  $\langle r \rangle_{6d} = 3.8a.u.$ ,  $\langle r \rangle_{7s} = 4.7a.u.$ ,  $\langle r \rangle_{7p} = 5.8a.u.$ ) this subshell is considered part of the core. The azimuthal symmetry for the virtuals is restricted to  $\ell \leq 4$  ( $g$  electron). This is justified by the decreasing contributions for  $vp vf$  and  $vd vg$  (see Table I). We provide the initial estimate for  $Z^*$ , using the nonrelativistic formula given in [23]. There are two parameters in this formula:  $\langle r \rangle$  and the principle quantum number. Our experience [15] shows that with the choice  $n = \ell + 1$ , we can get more than 90% of the correlation energy with a single virtual. For the biggest virtual contributors we used 3 sets of virtual spinors: the first set of virtuals is determined using  $\langle r \rangle$  for the  $7s$  orbital, the second set has the same  $\langle r \rangle$  and  $n = \ell + 2$ . With the third set we studied the effect of "deeper" virtuals,  $\langle r \rangle$  for the  $6s$  orbital, and  $n = \ell + 1$ . It turned out that the second and third sets have small net contributions (in  $Pa^-$ : 0.0016 eV for  $vf'$ ,  $vf''$ , 0.0038 eV for  $vp'$ ,  $vp''$  and 0.0058 eV for  $vd'$ ,  $vd''$ ).

### III. RESULTS

The electron affinity (EA) is determined as:  $EA = E_{\text{neutral}} - E_{\text{negative ion}}$ . The results for  $Pa$   $I$  ground state and  $Pa^-$  bound state are shown in Table I. It is seen that  $Pa^-$  is unbound at the MCDF level (one manifold), the same as for  $Ce^-$  [14],  $Pr^-$  [15] and  $U^-$  [13]. The biggest contributor to the unbinding is  $7s^2 \rightarrow (7p^2 + 7p\,vp + vp^2) = 0.1858$  eV, while the biggest binding (0.3652 eV) comes from  $7s \rightarrow (6d + vd)$  correlation. Those results are typical for the other Rare Earths that we studied [12–15]. Again as in other Rare Earths, the  $J$  for the most bound negative ion is given as  $J_{\text{negative ion}} = J_{\text{neutral}} - 1/2$ .

The energy correlation contributions are calculated using the intermediate normalization  $\langle \Phi, \Psi \rangle = 1$ , where  $\Phi$  is the MCDF, and  $\Psi$  is the CI wavefunction. Then the energy contribution for parent  $\chi_i$  is given by:

$$E_i = \frac{c_i}{c_\Phi} \langle \Phi | H | \chi_i \rangle \quad (1)$$

Here  $c_i$  is the CI configuration weight for the parent  $\chi_i$ , and  $c_\Phi$  is the combined weight for all MCDF parents (single manifold). All contributions for parents arising from the same nonrelativistic manifold are added in a single entry (see Table I).

The hyperfine structure (hfs) constants, the formulae are taken from [24], for the  $Pa^-$   $5f^2 6d 7s^2 7p$  bound state are  $A=741.3$  MHz,  $B=1309$  MHz. The MCDF (single manifold) values are  $A=699.6$  MHz,  $B=1061$  MHz, and the combined weight of all MCDF parents,  $c_\Phi$ , is 87%. We used  $\mu = 1.96$  for the nuclear magnetic dipole moment [25], and  $Q=1.720$  Barn for the nuclear electric quadrupole moment [26]. The nuclear spin for  $^{231}Pa$  is  $I=3/2$  [27]. The constant  $A$  scales as  $\mu$ , and  $B$  scales linearly with the value of the quadrupole moment  $Q$ .

The biggest error in our calculations is the neglect of the core-valence correlations. The error in the theoretical predictions could be as big as 60 meV, based on the recent experimental work on Strontium [28]. However, if we use  $Cs^-$  [29] as a reference point, we predict a smaller error,  $\sim 36$  meV. The  $J$  restrictions will introduce a smaller error than the missing

core-valence effects [13,15]. To fit our dimensional restrictions of 7000 eigenvectors, we removed all parents with coefficients less than 0.001 in magnitude, whose energy contribution is less than 0.0001 eV, before including more correlation configurations. In the process of removing small parents we keep all of them that are important for the hfs, even if their energy contribution and weight are small. This technique introduces an error below 10 meV, based on the energy of the removed parents. For this system we kept the matrix size under control with this technique only, but didn't use the Reduce method [19,24].

We also studied possible  $6d$  attachment to the threshold  $Pa\ 5f^26d^27s$  (attaching  $7s$  electron [12,14]), which is  $7000\ cm^{-1}$  above the ground state. Closing the  $7s$  shell is likely to give up to 0.5 eV lowering [12], which doesn't encourage us to believe in the  $6d$  attachment for this system. We examined possible  $Pa^-$  negative ion bound states ( $7p$  attachment) for other Js. At the MCDF level they are unbound by 0.3763 eV, and 0.4972 eV for  $J=5$  and  $J=7$  correspondingly, which can not be recovered by the  $7p$  attachment (less than 0.3 eV lowering, as suggested by this work).

What are the relativistic effects in those systems? First we observe that in all the systems:  $Ce^-$  [14],  $Pr^-$  [15],  $Th^-$  [12],  $U^-$  [13] and  $Pa^-$  [this work], the important quantum number to distinguish the negative ion bound states is  $J$ . Second, in Table II are shown the angular momentum sections with biggest contribution for the negative ions ( $np$  attachment) of Ce, Pr, Th, U and Pa. We see that for the most bound negative ion state the  $np$  electron has  $J=1/2$ . This is consistent with the experimental designation in [1].

Future work. As is seen from the discrepancies in the theoretical predictions for Lu negative ion ([30] vs [7,9]), more theoretical and experimental work is needed to resolve the discrepancies and study the important many-body effects in those systems.

In conclusion we predict one bound state for  $Pa$  negative ion, viz.  $Pa^- 5f^26d7s^27p\ J=6$ , which is bound to the  $Pa\ I$  neutral ground state by 0.222 eV, consistent with the relatively moderate yield of  $Pa^-$  ions [1].

TABLE I. Contributions (in eV) to the 7p EA of  $Pa^-$ . Dirac-Fock (DF) is given relative to  $Pa I$  DF. CI contributions are relative to their own DF. The radial functions are generated from  $5f^2[6d7s^2 + 6d^27s + 6d^3 + 6d7p^2 + 7s7p^2]$  for  $Pa I$ , and from  $5f^2[6d7s^27p + 6d^27s7p + 6d^37p + 6d7p^3 + 7s7p^3]$  for  $Pa^-$ . NA = not applicable.

Excitation	$Pa I$ J=11/2 , ground $5f^2 6d 7s^2$	$Pa^-$ J=6 $5f^2 6d 7s^2 7p$
DF dominant manifold	0	+0.0800
$7s \rightarrow 6d$	-0.2467	-0.5535
$\rightarrow vs$	-0.0038	-0.0054
$\rightarrow vd$	-0.0102	-0.0691
$\rightarrow vg$	-0.0309	-0.0285
$6d \rightarrow vs$	0	expected small
$\rightarrow vd$	-0.0074	-0.0405
$\rightarrow vg$	-0.0132	-0.0139
$7p \rightarrow vp$	NA	-0.0123
$\rightarrow vf$	NA	-0.0037
$7s^2 \rightarrow 6d^2$	-0.1272	-0.1451
$\rightarrow 7p^2$	-0.4358	-0.2151
$\rightarrow 6dvs$	0	expected small
$\rightarrow 6dvd$	-0.0141	-0.0109
$\rightarrow 6dvg$	0	expected small
$\rightarrow vs^2$	-0.0033	-0.0081
$\rightarrow vd^2$	-0.0006	-0.0013
$\rightarrow vg^2$	-0.0033	-0.0036
$\rightarrow vsvd$	0	expected small
$\rightarrow vdv g$	0	expected small
$\rightarrow 7pvp$	+0.0017	-0.0251

	$\rightarrow 7pvf$	0	0
	$\rightarrow vp^2$	-0.0013	-0.0123
	$\rightarrow vf^2$	-0.0083	-0.0092
	$\rightarrow vpvf$	0	0
$7s6d$	$\rightarrow 7p^2$	-0.0949	-0.0293
	$\rightarrow 7pvp$	-0.0028	-0.0188
	$\rightarrow 7pvf$	-0.1210	-0.1004
	$\rightarrow vpvf$	-0.0040	-0.0149
	$\rightarrow vp^2$	-0.0003	-0.0018
	$\rightarrow vf^2$	+0.0005	+0.0012
	$\rightarrow vsvd$	-0.0112	-0.0239
	$\rightarrow vsvg$	0	0
	$\rightarrow vdvf$	-0.0030	-0.0006
	$\rightarrow vs^2$	0	0
	$\rightarrow vd^2$	+0.0013	+0.0021
	$\rightarrow vg^2$	-0.0001	+0.0002
$6d7p$	$\rightarrow vpvf$	NA	-0.0405
	$\rightarrow vsvp$	NA	0
	$\rightarrow vsvf$	NA	-0.0002
	$\rightarrow vdvf$	NA	-0.0065
	$\rightarrow vgvf$	NA	-0.0001
	$\rightarrow vgvf$	NA	-0.0013
$7s7p$	$\rightarrow vsvp$	NA	-0.0243
	$\rightarrow vsvf$	NA	0
	$\rightarrow 6dvp$	NA	+0.0002
	$\rightarrow 6dvf$	NA	-0.0178
	$\rightarrow vdvf$	NA	-0.0052

$\rightarrow vdf$	NA	-0.0027
$\rightarrow vgvf$	NA	-0.0052
$\rightarrow vgvp$	NA	0
CI (total)	-1.1398	-1.4471
Breit	0.0	+0.005
EA	NA	0.222

TABLE II. The angular momentum sections with biggest contribution to the Dirac-Fock manifold for  $np$  attachment in  $Ce^-$ ,  $Pr^-$ ,  $Th^-$ ,  $U^-$  and  $Pa^-$ . The result for  $Pa^-$  is from this work. Sum of the percentages for each case gives the weight of the MCDF manifold.

system	$np_{1/2}$ attachment	%	$np_{3/2}$ attachment	%
$Ce^-$ 6p J=9/2 [14] EA=0.259 eV	$4f_{7/2} 5d_{3/2} 6s^2 6p_{1/2}$	2	$4f_{5/2} 5d_{5/2} 6s^2 6p_{3/2}$	2
	$4f_{5/2} 5d_{5/2} 6s^2 6p_{1/2}$	2	$4f_{5/2} 5d_{3/2} 6s^2 6p_{3/2}$	2
	$4f_{5/2} 5d_{3/2} 6s^2 6p_{1/2}$	74		
$Ce^-$ 6p J=7/2 [14] EA=0.147 eV	$4f_{5/2} 5d_{5/2} 6s^2 6p_{1/2}$	5	$4f_{7/2} 5d_{3/2} 6s^2 6p_{3/2}$	4
	$4f_{5/2} 5d_{3/2} 6s^2 6p_{1/2}$	1	$4f_{5/2} 5d_{5/2} 6s^2 6p_{3/2}$	11
			$4f_{5/2} 5d_{3/2} 6s^2 6p_{3/2}$	59
$Ce^-$ 6p J=7/2 <sub>1-st exc</sub> [14] EA=0.055 eV	$4f_{5/2} 5d_{3/2} 6s^2 6p_{1/2}$	56	$4f_{5/2} 5d_{5/2} 6s^2 6p_{3/2}$	7
			$4f_{5/2} 5d_{3/2} 6s^2 6p_{3/2}$	16
$Ce^-$ 6p J=5/2 [14] EA=0.105 eV	$4f_{5/2} 5d_{5/2} 6s^2 6p_{1/2}$	4	$4f_{5/2} 5d_{5/2} 6s^2 6p_{3/2}$	2
	$4f_{5/2} 5d_{3/2} 6s^2 6p_{1/2}$	72	$4f_{5/2} 5d_{3/2} 6s^2 6p_{3/2}$	5
$Ce^-$ 6p J=3/2 [14] EA=0.043 eV	$4f_{7/2} 5d_{3/2} 6s^2 6p_{1/2}$	1	$4f_{5/2} 5d_{5/2} 6s^2 6p_{3/2}$	2
	$4f_{5/2} 5d_{5/2} 6s^2 6p_{1/2}$	14		
	$4f_{5/2} 5d_{3/2} 6s^2 6p_{1/2}$	68		
$Pr^-$ 6p J=5 [15] EA=0.128 eV	$4f_{5/2} 4f_{7/2}^2 6s^2 6p_{1/2}$	8		
	$4f_{5/2}^2 4f_{7/2} 6s^2 6p_{1/2}$	31		
	$4f_{5/2}^3 6s^2 6p_{1/2}$	53		
$Pr^-$ 6p J=4 [15] EA=0.110 eV	$4f_{5/2} 4f_{7/2}^2 6s^2 6p_{1/2}$	8		
	$4f_{5/2}^2 4f_{7/2} 6s^2 6p_{1/2}$	31		
	$4f_{5/2}^3 6s^2 6p_{1/2}$	52		
$Th^-$ 7p J=7/2 [12] EA=0.042 eV	$6d_{3/2} 6d_{5/2} 7s^2 7p_{1/2}$	70	$6d_{3/2}^2 7s^2 7p_{3/2}$	19
$Th^-$ 7p J=5/2 [12]	$6d_{3/2} 6d_{5/2} 7s^2 7p_{1/2}$	1	$6d_{3/2} 6d_{5/2} 7s^2 7p_{3/2}$	1

EA=0.365 eV	$6d_{3/2}^2 7s^2 7p_{1/2}$	87		
$Th^-$ 7p J=3/2 [12]	$6d_{3/2} 6d_{5/2} 7s^2 7p_{1/2}$	20	$6d_{3/2} 6d_{5/2} 7s^2 7p_{3/2}$	7
EA=0.075 eV	$6d_{3/2}^2 7s^2 7p_{1/2}$	52	$6d_{3/2}^2 7s^2 7p_{3/2}$	2
	$6d_{5/2}^2 7s^2 7p_{1/2}$	3		
$Th^-$ 7p J=1/2 [12]	$6d_{3/2} 6d_{5/2} 7s^2 7p_{1/2}$	28	$6d_{3/2} 6d_{5/2} 7s^2 7p_{3/2}$	10
EA=0.088 eV	$6d_{3/2}^2 7s^2 7p_{1/2}$	24	$6d_{3/2}^2 7s^2 7p_{3/2}$	7
	$6d_{5/2}^2 7s^2 7p_{1/2}$	6	$6d_{5/2}^2 7s^2 7p_{3/2}$	3
$Pa^-$ 7p J=6	$5f_{5/2} 5f_{7/2} 6d_{3/2} 7s^2 7p_{1/2}$	2		
EA=0.222 eV	$5f_{5/2}^2 6d_{3/2} 7s^2 7p_{1/2}$	85		
$U^-$ 7p J=13/2 [13]	$5f_{5/2} 5f_{7/2}^2 6d_{3/2} 7s^2 7p_{1/2}$	1		
EA=0.175 eV	$5f_{5/2}^2 5f_{7/2} 6d_{3/2} 7s^2 7p_{1/2}$	16		
	$5f_{5/2}^3 6d_{5/2} 7s^2 7p_{1/2}$	1		
	$5f_{5/2}^3 6d_{3/2} 7s^2 7p_{1/2}$	68		

#### IV. ACKNOWLEDGEMENTS

We gratefully acknowledge the partial support for this work by the National Science Foundation, Grant No. 93-17828.

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