Ultra-cold antihydrogen atoms are of great scientific interest [1]. For example, they can be efficiently trapped for precise laser spectroscopy, enabling spectroscopic comparison with hydrogen. They are also ideal systems for direct measurement of gravitational acceleration of antimatter. To form antihydrogen below 1 K, it is crucial that the antiprotons be precooled before combining with the positrons [2]. It was proposed [3] that the antiprotons can be sympathetically cooled by transferring their energy to some precooled anions. These anions are cooled via laser cooling, where they absorb a laser photon and undergo electric dipole (E1) transitions to a bound state of opposite parity.

In an earlier paper [4], our research group proposed a new candidate for laser cooling, \( \text{La}^- \), in addition to \( \text{Os}^- \) [3, 5]. Comparisons were made [4] between these two anions. For example, the E1 transition in \( \text{La}^- \) has a smaller transition energy than that in \( \text{Os}^- \) (Fig. 1), but the upper state in \( \text{La}^- \) does not need to be repumped using a laser as will be needed for \( \text{Os}^- \). An ideal candidate anion would have only two bound states connected by an E1 transition. This is essentially true with \( \text{La}^- \) whose upper state decays almost entirely back to the ground state even though there are other lower states. The \( \text{Os}^- \) upper state, however, can decay into another state, necessitating the need to repump it to maintain efficient laser cooling.

One important consideration in laser cooling is the two-photon detachment loss. The upper state of the anion may absorb a second photon, which kicks off the excess electron, and become neutralized. \( \text{La}^- \) would not be a competitive candidate to \( \text{Os}^- \) for laser cooling if its loss due to photodetachment is much larger. For this reason, we decided to compare the upper state photodetachment cross sections of \( \text{La}^- \) and \( \text{Os}^- \) at their corresponding photon energies.

As shown in Fig. 1, the possible detachment channels for \( \text{La}^- \) and \( \text{Os}^- \) in laser cooling are:

\[
\begin{align*}
\text{La}^- &: 5d6s^26p^3 \, ^3D_1 \rightarrow 5d6s^2 \, ^2D_{3/2} + \epsilon l_j \\
\text{Os}^- &: 5d^66s^26p^6 \, ^6D_{5/2} \rightarrow 5d^66s^2 \, ^2F_{5/2} + \epsilon l_j
\end{align*}
\]

where \( \epsilon l_j \) denotes \( \epsilon s_{1/2} \) and \( \epsilon d_{3/2,5/2} \). The multiple detachment thresholds in \( \text{Os}^- \) are due to its large laser photon energy, 1.067 eV. The \( \text{Os} \) \( 5d^66s^2 \, ^2D_0, \, ^2D_1 \) states are omitted because neither can make a total \( J \) value that is accessible by an E1 transition after coupling with a free \( s \) or \( d \) electron.

In computing the cross sections for the above channels, we employ the relativistic configuration interaction (RCI) methodology. The wave functions for the anion bound state and the neutral thresholds were obtained by doing RCI calculations at the valence stage. The basis set consists of the reference configurations (Fig. 1) and correlation configurations that are one- or two-electron replacements of the reference configurations. The radial functions for the spinors occupied in the reference configurations are generated by the multiconfigurational Dirac-Fock (MCDF) code of Desclaux [8]. For those not occupied in the reference configurations, called virtual orbitals and denoted \( \epsilon l \), their radial functions are represented by the relativistic screened hydrogenic functions (RSH). The only adjustable parameter in a RSH function, the effective charge, \( Z^* \), is determined via energy minimization.

One merit of the RCI formalism is the basis set can be tailored to the atomic property under study. In a cross section calculation, the energy values of the anion states and the neutral states are taken from the measurements or calculations in literature (refer to the caption to Fig. 1). With energies being thus accounted for, in cross section calculations it is adequate for the wave function to be able to yield the converged \( LS \) compositions for an anion state, or a Landé \( g \) value that is in good agreement with the measurement in case of a neutral state. In addition, the radial space of the important configurations may need to be saturated by adding another virtual orbital of the same symmetry. In \( \text{La}^- \), introducing a second set of virtual orbitals lowers the total cross section by \( \sim 7\% \) while maintaining excellent gauge agreement \((\leq 1\%) \). The additional virtual \( p \) orbital helps saturate \( \text{La}^- 5d6s^2ep \), which is the only big contributor to the cross section other than the reference configuration. In \( \text{Os}^- \), the addition of the second virtual orbital changes the cross section very little \((<3\%) \). This is consistent
with the observation that the big contributors to the Os\(^-\) cross sections are exclusively the reference configurations.

Unlike the previous work [4], the 5d\(^2\) correlation was explicitly introduced in the basis set in this work. The near-degeneracy between the 5d and 6s electron manifests itself as the mixing of 5d\(^6\)6s\(^2\) of La\(^-\) 5d\(^6\)s\(^2\)6p\(^3\)D\(_1\) and the mixing of 5d\(^2\)6s\(^6\)p\(^3\)D\(_3/2\) in Os\(^-\) 5d\(^6\)6s\(^2\)6p\(^4\)D\(_3/2\). A full ab initio treatment would correlate explicitly both configurations by applying the same one- and two-electron replacements to them. For Os\(^-\), as discussed in the previous paper [4], it was thought that this would cause extensive second-order effects and lead to over-correlation of 5d\(^6\)6s\(^6\)p. The solution then was to omit the 5d\(^2\) correlation, but incorporate its effect to the wave function by shifting the related diagonal matrix elements. However, for the Os\(^-\) 6D\(_3/2\) odd state studied here, including the 5d\(^2\) correlation does not seem to cause problems. While the 5d\(^2\) correlation in 5d\(^6\)6s\(^2\)6p does introduce to 5d\(^6\)6s\(^6\)p the triple replacements 5d\(^2\) → 6s\(xl^2\) + 6sx\(xl\)'\(l\)' (xl denotes either a Dirac-Fock orbital \(nl\), or a virtual orbital \(vl\)), these replacements are going to be small. Experience has shown large triple replace-

ments are usually products of the large one- and two-electron replacements. The above 5d\(^3\) correlation can be viewed as a product of 5d → 6s and 5d\(^2\) → \(xl^2\) + 6sx\(xl\)'\(l\)', but 5d → 6s is small (e.g., contributes only several tens of meV to 5d\(^6\)6s in Os I). Therefore, we do not expect this 5d\(^3\) correlation to contribute much to 5d\(^6\)6s\(^6\)p. On the other hand, these 5d\(^3\) replacements are not applicable to 5d\(^6\)6s\(^2\)6p whose 6s subshell is already full. As a support to the above argument, after explicitly incorporating 5d\(^2\) correlation in the basis set, we obtain almost identical LS compositions as the previous calculation [4]. For the neutral states, the 5d\(^2\) correlation is also explicitly included and good agreements with the experimental Landé \(g\) values are obtained.

The 5d\(^2\) correlation produces a large number of basis functions, so we use the REDUCE method [9] to keep the basis size within the default 20 000 limit. Briefly, this method rotates the basis functions of a correlation configuration to maximize the number of functions that have zero matrix elements with the reference functions. These functions are then discarded, but those that have non-zero matrix elements are kept. With the REDUCE
method, a reduction of a factor of 20 is achievable.

The continuum state wave function is constructed by coupling the wave function of a free electron to that of a neutral state [10]. Assuming the angular part of the free electron’s wave function takes the same form as that of a bound electron, its radial function is numerically generated in a frozen-core Dirac-Fock potential, using a modified version [10] of the relativistic continuum wave solver code of Perger et al. [11, 12].

The cross section is calculated using [13]:

$$
\sigma = 4\pi^2 \alpha^2 \frac{d\sigma}{dE} = 8.067 \frac{d\sigma}{dE} \text{ (Mb),}
$$

where $$\alpha$$ is the fine-structure constant, $$a_0$$ is the radius of the first Bohr orbit, $$\frac{d\sigma}{dE}$$ is the differential oscillator strength for the E1 transition from the anion bound state to the continuum state. The $$\frac{d\sigma}{dE}$$ is evaluated using a modified version [14] of our code for bound states. This modified version has been used to reproduce the experimental photoelectron spectrum of Ce$^-$. [15].

It is known that the presence of resonances may produce pronounced features in the photoelectron spectrum. Therefore, it is important to mix the important resonance states into the wave function for the continuum state. An important resonance state, according to the Fano’s theory [16], should possess at least two properties: (1) it should be connected to the initial bound state by a strong E1 transition; (2) it should have a large mixing in the continuum state. In a previous work on HF [17], we implemented the Fano’s [16] and Mies’s [18] theory to incorporate the big resonance states. For La$^-$ and Os$^-$, however, analysis shows no big resonance state to be present. In the La$^-$ case, given the initial bound state 5$d_6s^26p^3D_1$, the potentially important resonance in a 6$p$ detachment would be 5$d^2p6s^2$. RCI calculations have shown (see Fig. 1) all the 5$d^2p6s^2$ states lie below the neutral ground state except for the $^1S_0$, $^1G_4$ state. Since the initial 5$d_6s^26p$ state is dominantly $^3D_1$, the transition to neither $^1S_0$ nor $^1G_4$ is E1 allowed. Similarly, for Os$^-$, the initial 5$d_6p6s^2$ is dominated by sextuplets (6$D_{2/2}$, 6$F_{3/2}$), but the potentially important resonance 5$d^2p6s$ can make at most a quartet. Due to this lack of big resonance states, no mixing of resonances into the continuum was made.

The calculated cross sections for La$^-$ and Os$^-$ are summarized in Table I. The cross section to each neutral threshold is the sum of all the relevant relativistic channels. As can be seen, we obtained very good gauge agreement for La$^-$ due to the careful selection of the 6$p$ radial functions [6] for La$^-$ 5$d_6s^26p$. The gauge agreement for Os$^-$ is not at the same level. However, our results for Os$^-$ are consistent with the order of estimates, 10$^{-17}$cm$^2$ (tens of Mb) [5] and 5$\times10^{-17}$cm$^2$ [19], both made by experimental data fitting.

As a conclusion, our calculations show the upper states in laser cooling of La$^-$ and Os$^-$ have very similar photodetachment cross sections. In other words, La$^-$ will have very similar two-photon detachment loss as Os$^-$ if used in laser cooling. Combined with its other merits [4], La$^-$ does make a promising candidate for laser cooling. It is our hope that this work will stimulate more experimental explorations in laser cooling of La$^-$, which can then be used to cool antiprotons to very low temperatures.

Acknowledgments

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\[\text{Table I: Photodetachment cross sections of the upper state of La}^-\text{and Os}^-\text{in laser cooling.}\]

<table>
<thead>
<tr>
<th>Anion</th>
<th>Upper Bound State</th>
<th>Neutral Threshold</th>
<th>Cross Section (Mb)</th>
</tr>
</thead>
<tbody>
<tr>
<td>La$^-$</td>
<td>5$d_6s^26p^3D_1$</td>
<td>5$d_6s^2$</td>
<td>34.4</td>
</tr>
<tr>
<td>Os$^-$</td>
<td>5$d_6s^26p^6D_{2/2}$</td>
<td>5$d_6p^6s^2^5D_4$</td>
<td>30.1</td>
</tr>
<tr>
<td>Os$^-$</td>
<td>5$d^2p6s^2$</td>
<td>5$d_6s^2^5D_2$</td>
<td>30.1</td>
</tr>
<tr>
<td>Os$^-$</td>
<td>5$d_6s^2$</td>
<td>5$d^2p6s^2$</td>
<td>5$d_6s^2^5D_1$</td>
</tr>
<tr>
<td>Os$^-$</td>
<td>5$d_6s^2$</td>
<td>5$d^2p6s^2$</td>
<td>5$d_6s^2$</td>
</tr>
<tr>
<td>total</td>
<td></td>
<td></td>
<td></td>
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