DeKock, Strikwerda, and Yu showed in 2012 how an atom’s “effective” atomic size, \( r_e \), relates to its average valence ionization energy [1]. The published values of \( r_e \) correlate well with other measures of atomic size. These ideas can be applied to cations as well to obtain radius ratios. To obtain such a simplified equation, we note that successive ionization energies of atoms roughly follow an arithmetic progression. If this arithmetic progression is assumed, we can derive the ratio

\[
\frac{r_e}{r_e^{++}} = \sqrt{\frac{N(N+1) - \gamma(N+1)}{(N-\gamma)(N+1)}}
\]

where \( N \) is the number of valence electrons in the neutral atom, and \( \gamma \) refers to the charge on the cation. Neutral to cation radius ratios were calculated using this formula and compared to actual radius ratios from theoretical radii.

The quantum chemistry software package GAMESS [2] was used to calculate the theoretical radii. A total of six theoretical radii were studied, and we report results of two of these radii here. These are \( r_{\text{max}} \), the maximum of the volume weighted radial probability distribution function, and \(<r>\), the expectation value of the radius. Radial calculations were done for neutral atoms and their ions across the periodic table from H through Kr (atomic number 1-36) minus the transition metal elements. A subset of our results are shown here for the valence orbital cations of Ne. Our predicted values for the ratio of neutral to cation radius were shown to correlate best with \( r_{\text{max}} \) for Ne as the \(<r>\) ratio was too large for each cation. Similar results were obtained for other elements.

<table>
<thead>
<tr>
<th>Species</th>
<th>( r_{\text{max}} )</th>
<th>(&lt;r&gt;)</th>
<th>Predicted</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ne(^+)</td>
<td>1.05</td>
<td>1.10</td>
<td>1.05</td>
</tr>
<tr>
<td>Ne(^2+)</td>
<td>1.08</td>
<td>1.20</td>
<td>1.11</td>
</tr>
<tr>
<td>Ne(^3+)</td>
<td>1.16</td>
<td>1.30</td>
<td>1.15</td>
</tr>
<tr>
<td>Ne(^4+)</td>
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<td>1.38</td>
<td>1.20</td>
</tr>
<tr>
<td>Ne(^5+)</td>
<td>1.27</td>
<td>1.45</td>
<td>1.25</td>
</tr>
</tbody>
</table>

Our work is also directly related to atomic polarizability, \( \alpha \). Polarizability is a fundamental property of atoms that is related to van der Waals interactions. It has been shown to correlate with the cube of atomic size. Cubing our radius ratio equation results in an equation that can be used to estimate the ratio of polarizabilities of a neutral atom compared to its cation:

\[
\frac{\alpha}{\alpha^{++}} = \left(\frac{N(N+1) - \gamma(N+1)}{(N-\gamma)(N+1)}\right)^{\frac{3}{2}}
\]

We have completed theoretical studies of polarizability ratios using this equation, compared them to experimental polarizabilities, and found reasonable agreement between the two methods. There has been recent interest in polarizability [3,4], and our work can provide new insight into this property and its relationship to atomic size and ionization energy.

This research experience has been a great benefit to me. I enjoyed being able to combine chemistry with mathematics, physics, and computer science on a project that explores the foundations of the electronic structure of atoms. I also have gained valuable scientific writing and presentation experience that will benefit me in my future academic and professional work. I am very grateful for this opportunity.

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