Solvation of Isoelectronic Halide and Alkali Metal Ions by Noble Gas Atoms

by

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Abstract

Alkali metal cations ($M^+ = \text{Li}^+, \text{Na}^+, \text{K}^+, \text{and Rb}^+$), as well as their corresponding isoelectronic atomic anions ($X^- = \text{H}^-, \text{F}^-, \text{Cl}^-, \text{and Br}^-$) were solvated with argon atoms (i.e., $M^+\text{Ar}_n$ and $X^-\text{Ar}_n$ where $n=1–6$). Full geometry optimizations were performed using the MP2 electronic structure method with a series of correlation consistent basis sets augmented with diffuse functions on argon and the anions (aug-cc-pV$XZ$) and weighted core valence basis sets were used for the cations (cc-pwCV$XZ$) that include the appropriate pseudopotentials for K$^+$ and Rb$^+$ (cc-pwCV$XZ$-PP). The basis sets for a particular cluster are, hereafter, simply denoted as $XZ$ where $X = T, Q, \text{or } 5$. A series of single point energies and scans were also performed using MP2 and CCSD(T) methods with basis sets as large as 5$Z$ for smaller clusters to gauge basis set and electron correlation effects. These computations were performed to explore similarities and differences between the isoelectronic cation and anion pairs ($\text{Li}^+ \text{vs. H}^-, \text{Na}^+ \text{vs. F}^-, \text{K}^+ \text{vs. Cl}^-, \text{and Rb}^+ \text{vs. Br}^-$).
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1 Introduction

Ion solvation is an area of much interest today due to its prevalence in many areas of scientific research, such as biochemistry (i.e., specific macromolecular transport systems such as ion channels and pumps) and electrochemistry (i.e., electroplating). The most fundamental aspects of ion solvation can be probed with the formation of small clusters in which a single atomic ion is “surrounded” by a small number of isotropic, nonpolar solvent atoms such as noble gas atoms (i.e., He, Ne, Ar, etc.). As such, a variety of experimental and computational studies have been carried out to characterize the interactions of noble gas atoms with an alkali metal or alkaline earth metal atomic cation (i.e., $M^+(\text{Ng})_n$ or $M^{2+}(\text{Ng})_n$).\textsuperscript{1–21}

Over the past two decades, several theoretical investigations have been performed to specifically characterize the interactions among Li$^+$ and Na$^+$ alkali metal cations solvated with Ar atoms.\textsuperscript{22–26} Such characterizations have led to the identification of various low energy configurations for the Li$^+$Ar$^+_n$ and Na$^+$Ar$^+_n$ systems. In 2004, Szymczak et al.\textsuperscript{22} utilized the MP2 electronic structure method in conjunction with a triple-$\zeta$ basis set to investigate the structures and properties of the Li$^+$Ar$^+_n$ system where $n=1$–6. Typical symmetric configurations (i.e., configurations defined by VSEPR Theory) were reported for low energy configurations for each cluster except Li$^+$Ar$_5$, in which the low energy configuration was reported to have an atypical, $C_{4v}$ symmetry. More recently, Prudente et al.\textsuperscript{23} reported low energy configurations for optimized Li$^+$Ar$^+_n$ ($n=2$–10) clusters using the MP2 method in conjunction with a quadruple-$\zeta$ basis set. For smaller Li$^+$Ar$^+_n$ clusters (i.e., $n=1$–6) the low energy configurations reported by Prudente et al. show good agreement with those reported by Szymczak et al. except for Li$^+$Ar$_2$, in which a bent configuration with $C_{2v}$ symmetry was reported by Prudente et al. and a linear configuration with $D_{\infty h}$ symmetry was reported by Szymczak et al.

Several similar investigations have been performed to characterize the Na$^+$Ar$_n$...
system, revealing some agreement among low energy configurations with the Li$^+$Ar$_n$ investigations.\textsuperscript{24–26} Two comparable investigations were performed in 2004 with aims to characterize interactions between Na$^+$ and Ar.\textsuperscript{24,25} Nagata \textit{et al.}\textsuperscript{24} utilized the MP2 method in conjunction with a triple-$\zeta$ basis set to perform geometry optimizations on Na$^+$Ar$_n$ clusters where $n=1–10$. Typical symmetric configurations were reported for the Na$^+$Ar$_2$ and Na$^+$Ar$_6$ clusters (i.e., $D_{\infty h}$ and $O_h$ symmetries, respectively), whereas atypical configurations were reported for Na$^+$Ar$_n$ where $n=3$, 4 and 5. Similarly, Giju \textit{et al.}\textsuperscript{25} utilized the MP2 method in conjunction with a triple-$\zeta$ basis set to identify low energy configurations for Na$^+$Ar$_n$ clusters where $n=1–8$. In contrast to Nagata \textit{et al.}, two low-energy configurations were reported for Na$^+$Ar$_n$ clusters where $n=2$, 3 and 4. As seen in the previously mentioned investigation performed by Nagata \textit{et al.}, typical and atypical configurations were identified as low energy configurations, though additional atypical configurations are reported by Giju \textit{et al.} (i.e., $C_{2v}$ symmetry for Na$^+$Ar$_2$ and $C_{3v}$ symmetry for Na$^+$Ar$_3$). Additionally, a similar investigation of the Na$^+$Ar$_n$ system was performed by Rhouma \textit{et al.}\textsuperscript{26} in 2006, in which atomistic potentials fitted to reproduce \textit{ab initio} calculations performed at the coupled-cluster level on smaller clusters were used to investigate structures and stabilities of Na$^+$Ar$_n$ ($n=1–54$) clusters. In comparing low energy configurations with the previous two studies, similar typical and atypical configurations were reported by Rhouma \textit{et al.} for Na$^+$Ar$_n$ clusters where $n=1–8$. Comparable to Giju \textit{et al.}, two low energy configurations were reported for Na$^+$Ar$_n$ clusters where $n=2$, 3 and 4. A slight deviation in reported symmetries appears for Na$^+$Ar$_4$, where competition takes place between the planar D$_{4h}$ and the C$_{2v}$ configuration rather than between the C$_{2v}$ and T$_d$ configuration reported by Giju \textit{et al.}

This present study aims to build upon these prior works by using higher levels of theory (i.e., MP2 and CCSD(T) methods in conjunction with quadruple-$\zeta$ basis sets) to perform a more extensive exploration of the Li$^+$Ar$_n$ and Na$^+$Ar$_n$ systems, as well as to expand the exploration to include the K$^+$Ar$_n$ and Rb$^+$Ar$_n$ systems in order to provide a more thorough characterization of interactions between alkali metal cations and Ar atoms. Additionally, this research seeks to provide characterization of interac-
tions between halide ions and Ar atoms. Few investigations have been performed on halide ions solvated by noble gas atoms.\textsuperscript{27–33} Moreover, to our knowledge, a systematic investigation has yet to be performed on metal cations and their corresponding isoelectronic anions. Our goal is to thoroughly describe the relationship between the structures and energetics of isoelectronic alkali metal cations and halide ions solvated with Ar atoms.
2 Computational Methods

Full geometry optimizations were performed upon the $M^+\text{Ar}_n$ system, (where $M^+$=Li$^+$, Na$^+$, K$^+$, Rb$^+$ and $n$=1–6) and the $X^-\text{Ar}_n$ system, (where $X^-$=H$^-$, F$^-$, Cl$^-$, Br$^-$ and $n$=1–6), using the MP2 method$^{34}$ with a series of correlation consistent basis sets augmented with diffuse functions on Ar, H$^-$, F$^-$, Cl$^-$ and Br$^-$ (aug-cc-pVXZ)$^{35–37}$ and weighted core valence correlation consistent basis sets were used for Li$^+$, Na$^+$, K$^+$ and Rb$^+$ (cc-pwCVXZ)$^{38}$ that include the appropriate pseudopotentials for K$^+$ and Rb$^+$ (cc-pwCVXZ-PP)$^{39}$, hereafter simply denoted as XZ where $X=$T or Q. Single point CCSD(T)$^{40,41}$ energy computations were performed upon the MP2/QZ optimized structures with the same basis set. An additional series of single point energy computations were performed with the MP2 and CCSD(T) method to scan over the interatomic distances in $M^+\text{Ar}_1$ and $X^-\text{Ar}_1$ clusters using TZ and the analogous QZ and 5Z basis sets. Similarly, relaxed angular scans of $M^+\text{Ar}_2$ and $X^-\text{Ar}_2$ clusters were performed with the same methods and basis sets to compare electron correlation and basis set effects between the anion and cation systems.

Electronic binding energies ($E_{\text{bind}}$) are determined for every structure by comparing the total electronic energy of each cluster ($M^+\text{Ar}_n$ or $X^-\text{Ar}_n$) to those of the isolated fragments $n$ Ar atoms and either an $M^+$ or $X^-$ ion). Similarly, the sequential binding energy for a cluster with $n$ Ar atoms is defined by comparing its binding energy to $E_{\text{bind}}$ for the corresponding cluster with one less Ar atom ($\Delta E_{\text{bind}}$=$E_{\text{bind}}[M^+\text{Ar}_n]$–$E_{\text{bind}}[M^+\text{Ar}_{n-1}]$) or $\Delta E_{\text{bind}}$=$E_{\text{bind}}[X^-\text{Ar}_n]$–$E_{\text{bind}}[X^-\text{Ar}_{n-1}]$). Note that for $n$=1 $E_{\text{bind}}$=$\Delta E_{\text{bind}}$.

All MP2 geometry optimizations were carried out with Gaussian16.$^{42}$ Additionally, all single point energy computations and scans using the CCSD(T) method were performed with Molpro2015.1$^{43}$. Default frozen core approximation was used for the $X^-\text{Ar}_n$ systems, whereas for the $M^+\text{Ar}_n$ systems frozen core was manually specified. All electrons were correlated for H$^-$ and Li$^+$, whereas the 1s-like orbital was frozen.
for F\(^-\) and Na\(^+\). The 1s2s2p-like orbitals were frozen for Cl\(^-\) and the 10MDF effective core potential was utilized for K\(^+\).\(^{44}\) Similarly, the 1s2s2p3s3p-like orbitals were frozen for Br\(^-\) and the 28MDF effective core potential was utilized for Rb\(^+\).\(^{44}\) The 28MDF effective core potential for Br\(^-\)\(^{45}\) was tested and compared to freezing the 1s2s2p3s3p-like orbitals which led to the decision to use frozen core approximation for Br\(^-\). Details of this analysis can be found in the appendix.
# 3 Results and Discussion

All unique configurations for the $\text{M}^+\text{Ar}_n$ and $\text{X}^-\text{Ar}_n$ clusters identified in this study are depicted in Figures 1–4 at the MP2/QZ level of theory. Each figure shows the $\text{M}^+\text{Ar}_n$ clusters on the left and the $\text{X}^-\text{Ar}_n$ clusters on the right for their respective central ions and number of Ar atoms. All configurations are individually labeled with the appropriate central ion and point group. For $n \geq 2$, two low-energy minima were found for most clusters. Only one minimum was identified for $\text{Na}^+\text{Ar}_6$ and for $\text{Li}^+\text{Ar}_n$ when $n=2, 3, 4$ and $6$. The configurations reported here for the $\text{Li}^+\text{Ar}_n$ and $\text{Na}^+\text{Ar}_n$ clusters are consistent with those previously reported.\textsuperscript{22,24,25}

The structures observed for these clusters include the high-symmetry fundamental geometries familiar to most chemists from VSEPR Theory\textsuperscript{46} that effectively place the atomic ions in the center of a solvation shell of Ar atoms. As defined in Figure 5, the linear ($D_{\infty h}$ for $n=1$ and 2), trigonal planar ($D_{3h}$ for $n=3$), tetrahedral ($T_d$ for $n=4$) and octahedral ($O_h$ for $n=6$) optimized structures are defined by a single bond length while the trigonal bipyramidal geometry ($D_{3h}$ for $n=5$) requires only one additional bond distance. Most of the other structures are closely related distortions of these basic shapes: bent ($C_{2v}$ for $n=2$), t-shaped and pyramidal ($C_{2v}$ and $C_{3v}$ for $n=3$), see-saw ($C_{2v}$ for $n=4$) and square pyramidal ($C_{4v}$ for $n=5$). The specification of these structures requires additional geometrical parameters (up to two unique bond lengths and two unique bond angles). The optimized geometrical parameters for each structure are reported in the Appendix. For $n=6$, an interesting and completely novel $C_{2v}$ minimum has also been identified for every ion examined except $\text{Li}^+$ and $\text{Na}^+$. This $C_{2v}$ structure appears to be derived from a pentagonal bipyramid with a vacant equatorial position in the same manner a see-saw structure is derived from a trigonal bipyramid.
Figure 1: $M^+\text{Ar}_n$ and $X^-\text{Ar}_n$ clusters and their respective configurations labeled with the appropriate central ion and point group at the MP2/QZ level of theory.
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<thead>
<tr>
<th>M$^+$Ar$_5$</th>
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<td>H$^+$</td>
</tr>
<tr>
<td>(D$_3h$)</td>
<td>(C$_{3v}$)</td>
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<tr>
<td>Na$^+$</td>
<td>F$^-$</td>
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<tr>
<td>(C$_{3v}$)</td>
<td>(C$_{2v}$)</td>
</tr>
<tr>
<td>K$^+$</td>
<td>Cl$^-$</td>
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<td>(C$_{2v}$)</td>
<td>(C$_{2v}$)</td>
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<td>(C$_{2v}$)</td>
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<table>
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<tr>
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<td>(C$_{3v}$)</td>
</tr>
<tr>
<td>Na$^+$</td>
<td>F$^-$</td>
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<tr>
<td>(C$_{3v}$)</td>
<td>(C$_{2v}$)</td>
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<td>Cl$^-$</td>
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<td>(C$_{2v}$)</td>
<td>(C$_{2v}$)</td>
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<td>Br$^-$</td>
</tr>
<tr>
<td>(C$_{2v}$)</td>
<td>(C$_{2v}$)</td>
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</table>

Figure 2: M$^+$Ar$_n$ and X$^-$.Ar$_n$ clusters and their respective configurations labeled with the appropriate central ion and point group at the MP2/QZ level of theory.
Figure 3: $\text{M}^+\text{Ar}_n$ and $\text{X}^-\text{Ar}_n$ clusters and their respective configurations labeled with the appropriate central ion and point group at the MP2/QZ level of theory.
<table>
<thead>
<tr>
<th>$M^+\text{Ar}_n$</th>
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<td>$\langle C_{3v} \rangle$</td>
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<tr>
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<td><strong>F</strong></td>
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<tr>
<td><img src="image3" alt="Na^+" /></td>
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<td>$\langle C_{3v} \rangle$</td>
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<td><strong>Br</strong></td>
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<tr>
<td>$\langle C_{3v} \rangle$</td>
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</tbody>
</table>

Figure 4: $M^+\text{Ar}_n$ and $X^-\text{Ar}_n$ clusters and their respective configurations labeled with the appropriate central ion and point group at the MP2/QZ level of theory.
Figure 5: Unique geometrical parameters defined (interatomic distances (R) in Å and angles (A) in degrees) in relation to the corresponding point groups of each $M^+\text{Ar}_n$ and $X^-\text{Ar}_n$ configuration.
Tables 1–4 report the geometrical parameters defined in Figure 5, including various intermolecular distances (R in Å), angles (A in degrees), and point groups for the M+Arₙ and X−Arₙ clusters at the MP2/QZ level of theory. Figure 6 provides a visual representation of the intermolecular distances reported in Tables 1–4. Intermolecular distances are reported for each M+Arₙ and X−Arₙ cluster, in order of increasing ion size and number of Ar atoms. As you move down Group 1 on the periodic table (i.e., Li to Rb), intermolecular distances increase. The same trend can be seen for the anion clusters, except for H−Arₙ where intermolecular distances are longer than those for F−Arₙ. The longest intermolecular distance can be seen within the C₄ᵥ square pyramidal structure (i.e., R₁) for all M+Arₙ and X−Arₙ clusters except Na+Arₙ where the longest intermolecular distance presents in the Na+Ar₆ O₆ octahedra structure.

Tables 5–8 report binding energies (only for applicable M+Arₙ and X−Arₙ clusters) for all configurations depicted in Figures 1–4 at the MP2/QZ and CCSD(T)/QZ levels of theory. The binding energies represent how strongly clusters are bound, whereas ∆E represents the intrinsic energetics for similar clusters. All clusters are bound, with X−Arₙ clusters being less bound than M+Arₙ clusters. This can be seen with the strongest bound clusters, Li+Arₙ, and the weakest bound clusters, H−Arₙ.

For example, at the CCSD(T)/QZ level of theory, the binding energy of Li+Ar₄(T₆) is −28.05 kcal mol⁻¹, whereas the binding energy of H−Ar₄(T₆) is −3.07 kcal mol⁻¹. The deviations in binding energy among isoelectronic clusters decrease as you move down the periodic table. For example, the binding energy of Rb+Ar₄(T₆) is −12.01 kcal mol⁻¹, whereas the binding energy of Br−Ar₄(T₆) is −4.84 kcal mol⁻¹. Generally, ∆E increases between configurations as you move down the periodic table. The exception to this pattern is seen with H−Arₙ clusters. Additionally, when comparing isoelectronic pairs, M+Arₙ clusters have smaller relative energies than X−Arₙ clusters.

Figure 7 depicts the sequential binding energies for all M+Arₙ and X−Arₙ clusters at the CCSD(T)/QZ level of theory. The sequential binding energies represent the change in binding energy as the number of Ar atoms is increased from 1 to 6 for the M+Arₙ and X−Arₙ clusters. Similar to the previous trends in geometrical parameters and binding energies, the deviations in sequential binding energy are largest between
Li$^+$Ar$_n$ and H$^-$Ar$_n$ clusters and decrease as you move down the periodic table, with the smallest deviations appearing between Rb$^+$Ar$_n$ and Br$^-$Ar$_n$ clusters.

Table 1: Geometrical parameters including various intermolecular distances (R in Å), angles (A in degrees), and point groups for the M$^+$Ar$_n$ and X$^-$Ar$_n$ clusters at the MP2/QZ level of theory.

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Table 2: Geometrical parameters including various intermolecular distances (R in Å), angles (A in degrees), and point groups for the $\text{M}^+\text{Ar}_n$ and $\text{X}^-\text{Ar}_n$ clusters at the MP2/QZ level of theory.

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<th>Cluster</th>
<th>$n$</th>
<th>Symmetry</th>
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<th>$R_2$</th>
<th>$R_3$</th>
<th>$A_1$</th>
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Table 3: Geometrical parameters including various intermolecular distances (R in Å), angles (A in degrees), and point groups for the M$^+$Ar$_n$ and X$^-$Ar$_n$ clusters at the MP2/QZ level of theory.

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Table 4: Geometrical parameters including various intermolecular distances (R in Å), angles (A in degrees), and point groups for the \( \text{M}^+\text{Ar}_n \) and \( \text{X}^-\text{Ar}_n \) clusters at the MP2/QZ level of theory.

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Figure 6: Intermolecular distances (R in Å) for the $M^+\text{Ar}_n$ and $X^-\text{Ar}_n$ clusters at the MP2/QZ level of theory.
Table 5: Electronic binding energies ($E_{\text{bind}}$ in kcal mol$^{-1}$) and relative electronic energies ($\Delta E$ in kcal mol$^{-1}$) for the $M^+\text{Ar}_n$ and $X^-\text{Ar}_n$ clusters at both the MP2/QZ and CCSD(T)/QZ level of theory.

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Table 6: Electronic binding energies ($E_{\text{bind}}$ in kcal mol$^{-1}$) and relative electronic energies ($\Delta E$ in kcal mol$^{-1}$) for the M$^+$Ar$_n$ and X$^-$Ar$_n$ clusters at both the MP2/QZ and CCSD(T)/QZ level of theory.

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Table 7: Electronic binding energies ($E_{bind}$ in kcal mol$^{-1}$) and relative electronic energies ($\Delta E$ in kcal mol$^{-1}$) for the M$^+$Ar$_n$ and X$^-$Ar$_n$ clusters at both the MP2/QZ and CCSD(T)/QZ level of theory.

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Table 8: Electronic binding energies ($E_{\text{bind}}$ in kcal mol$^{-1}$) and relative electronic energies ($\Delta E$ in kcal mol$^{-1}$) for the $M^+\text{Ar}_n$ and $X^-\text{Ar}_n$ clusters at both the MP2/QZ and CCSD(T)/QZ level of theory.

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Figure 7: Sequential binding energies (E_n in kcal mol⁻¹) for the M⁺Ar_n and X⁻Ar_n (where n=1–6) clusters at the CCSD(T)/QZ level of theory.
4 Conclusions

This study provides a thorough characterization of the $M^+Ar_n$ and $X^-Ar_n$ systems via full geometry optimizations and vibrational frequency computations with sophisticated \textit{ab initio} levels of theory. As an extension of the previous literature\textsuperscript{22–26} we identified low-energy configurations for Li$^+Ar_n$ and Na$^+Ar_n$ systems where $n=1–6$, as well as for the analogous K$^+Ar_n$ and Rb$^+Ar_n$ systems. Additionally, we were able to fully characterize the corresponding isoelectronic anion clusters (i.e., H$^-Ar_n$, F$^-Ar_n$, Cl$^-Ar_n$, and Br$^-Ar_n$, respectively). Generally, the low-energy minima for each system agree with those reported in the previous literature. Consistent with patterns seen among the Li$^+Ar_n$ and Na$^+Ar_n$ investigations, two low-energy minima were identified for most clusters where $n \geq 2$, whereas only one minimum was identified for Na$^+Ar_6$ and for Li$^+Ar_n$ where $n=2$, 3, 4 and 6.

A general trend is seen among solvated structures for all $M^+Ar_n$ and $X^-Ar_n$ clusters, where the lowest energy configurations were in agreement across most systems. Deviations in lowest-energy configurations are seen among Li$^+Ar_n$ where $n=2$, 3, 4 and 6 and Na$^+Ar_6$ in comparison to the other $M^+Ar_n$ and $X^-Ar_n$ configurations. Additional low energy configurations for larger clusters (i.e., $M^+Ar_n$ and $X^-Ar_n$ where $n=5$ and 6) not seen in previous literature or found within the Li$^+Ar_n$ and Na$^-Ar_n$ were identified and reported within this investigation. The lowest energy configurations are typically those that show favorable Ar-Ar attractions (i.e., atypical configurations).

In general, $M^+Ar_n$ clusters are more strongly bound than $X^-Ar_n$ clusters, with deviations in $E_{\text{bind}}$ among isoelectronic clusters decreasing with progression down the periodic table (i.e., Li to Rb and H to Br). Additionally, $M^+Ar_n$ clusters have smaller relative energies than $X^-Ar_n$ clusters. $\Delta E$ generally increases between low-energy configurations decreasing with progression down the periodic table, with the exception appearing for H$^-Ar_n$ clusters.

The thorough characterization of the $M^+Ar_n$ and $X^-Ar_n$ isoelectronic systems
found within this investigation will provide valuable information on similar systems in future experimental and theoretical investigations of explicit microsolvation of ions by noble gas atoms.
References


ionic centers in rare gas clusters: The (Ne)$_n$H$^-$ and (Ne)$_{n+1}$ systems. http://dx.doi.org/10.1063/1.1599343.


Appendix
Table A1: Cartesian coordinates in Angstroms (Å) for the $C_{\infty v}$ optimized geometry
of Li$^+$Ar at the MP2/TZ level of theory.

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Table A2: Cartesian coordinates in Angstroms (Å) for the $D_{\infty h}$ optimized geometry
of Li$^+$Ar$_2$ at the MP2/TZ level of theory.

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</tr>
<tr>
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Table A3: Cartesian coordinates in Angstroms (Å) for the $D_{3h}$ optimized geometry
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Table A4: Cartesian coordinates in Angstroms (Å) for the $T_d$ optimized geometry of Li$^+$Ar$_4$ at the MP2/TZ level of theory.

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Table A5: Cartesian coordinates in Angstroms (Å) for the $C_{4v}$ optimized geometry of Li$^+$Ar$_5$ at the MP2/TZ level of theory.

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Table A6: Cartesian coordinates in Angstroms (Å) for the $D_{3h}$ optimized geometry of Li$^+$Ar$_5$ at the MP2/TZ level of theory.

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Table A7: Cartesian coordinates in Angstroms (Å) for the $O_h$ optimized geometry of Li$^+$Ar$_6$ at the MP2/TZ level of theory.

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<tr>
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Table A8: Cartesian coordinates in Angstroms (Å) for the $C_{\infty v}$ optimized geometry of Na$^+$Ar at the MP2/TZ level of theory.

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Table A9: Cartesian coordinates in Angstroms (Å) for the $D_{\infty h}$ optimized geometry of Na$^+$Ar$_2$ at the MP2/TZ level of theory.

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Table A10: Cartesian coordinates in Angstroms (Å) for the $C_{2v}$ optimized geometry of Na$^+$Ar$_2$ at the MP2/TZ level of theory.

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Table A11: Cartesian coordinates in Angstroms (Å) for the C$_{3v}$ optimized geometry of Na$^+$Ar$_3$ at the MP2/TZ level of theory.

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Table A12: Cartesian coordinates in Angstroms (Å) for the C$_{2v}$ optimized geometry of Na$^+$Ar$_3$ at the MP2/TZ level of theory.

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Table A13: Cartesian coordinates in Angstroms (Å) for the C$_{2v}$ optimized geometry of Na$^+$Ar$_4$ at the MP2/TZ level of theory.

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Table A14: Cartesian coordinates in Angstroms (Å) for the $T_d$ optimized geometry of Na$^+$Ar$_4$ at the MP2/TZ level of theory.

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Table A15: Cartesian coordinates in Angstroms (Å) for the $C_{4v}$ optimized geometry of Na$^+$Ar$_5$ at the MP2/TZ level of theory.

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Table A16: Cartesian coordinates in Angstroms (Å) for the $D_{3h}$ optimized geometry of Na$^+$Ar$_5$ at the MP2/TZ level of theory.

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Table A17: Cartesian coordinates in Angstroms (Å) for the $O_h$ optimized geometry of Na$^+$Ar$_6$ at the MP2/TZ level of theory.

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Table A18: Cartesian coordinates in Angstroms (Å) for the $C_{\infty v}$ optimized geometry of K$^+$Ar at the MP2/TZ level of theory.

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Table A19: Cartesian coordinates in Angstroms (Å) for the $C_{2v}$ optimized geometry of K$^+$Ar$_2$ at the MP2/TZ level of theory.

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Table A20: Cartesian coordinates in Angstroms (Å) for the $D_{\infty h}$ optimized geometry of K$^+$Ar$_2$ at the MP2/TZ level of theory.

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Table A21: Cartesian coordinates in Angstroms (Å) for the C\textsubscript{3v} optimized geometry of K\textsuperscript{+}Ar\textsubscript{3} at the MP2/TZ level of theory.

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Table A22: Cartesian coordinates in Angstroms (Å) for the C\textsubscript{2v} optimized geometry of K\textsuperscript{+}Ar\textsubscript{3} at the MP2/TZ level of theory.

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Table A23: Cartesian coordinates in Angstroms (Å) for the C\textsubscript{2v} optimized geometry of K\textsuperscript{+}Ar\textsubscript{4} at the MP2/TZ level of theory.

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Table A24: Cartesian coordinates in Angstroms (Å) for the $T_d$ optimized geometry of $K^+\text{Ar}_4$ at the MP2/TZ level of theory.

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Table A25: Cartesian coordinates in Angstroms (Å) for the $C_{4v}$ optimized geometry of $K^+\text{Ar}_5$ at the MP2/TZ level of theory.

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Table A26: Cartesian coordinates in Angstroms (Å) for the D$_{3h}$ optimized geometry of K$^+$Ar$_5$ at the MP2/TZ level of theory.

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<td>0.000000</td>
<td>3.207295</td>
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<tr>
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<td>0.000000</td>
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Table A27: Cartesian coordinates in Angstroms (Å) for the C$_{2v}$ optimized geometry of K$^+$Ar$_6$ at the MP2/TZ level of theory.

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<td>K</td>
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<td>Ar</td>
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<td>Ar</td>
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<td>0.000000</td>
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<tr>
<td>Ar</td>
<td>0.239735</td>
<td>0.165662</td>
<td>3.038227</td>
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<td>Ar</td>
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</tr>
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Table A28: Cartesian coordinates in Angstroms (Å) for the $O_h$ optimized geometry of K$^+$Ar$_6$ at the MP2/TZ level of theory.

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</table>

Table A29: Cartesian coordinates in Angstroms (Å) for the $C_{\infty v}$ optimized geometry of Rb$^+$Ar at the MP2/TZ level of theory.

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<td>Ar</td>
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Table A30: Cartesian coordinates in Angstroms (Å) for the $C_{2v}$ optimized geometry of Rb$^+$Ar$_2$ at the MP2/TZ level of theory.

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Table A31: Cartesian coordinates in Angstroms (Å) for the $D_{\infty h}$ optimized geometry of Rb$^+$Ar$_2$ at the MP2/TZ level of theory.

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<tr>
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<tr>
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Table A32: Cartesian coordinates in Angstroms (Å) for the $C_{3v}$ optimized geometry of Rb$^+$Ar$_3$ at the MP2/TZ level of theory.

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</thead>
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<td>Ar</td>
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<td>−1.038695</td>
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<tr>
<td>Ar</td>
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<td>−1.114242</td>
<td>−1.038695</td>
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Table A33: Cartesian coordinates in Angstroms (Å) for the $C_{2v}$ optimized geometry of Rb$^+$Ar$_3$ at the MP2/TZ level of theory.

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<td>Ar</td>
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<td>Ar</td>
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<td>1.181727</td>
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<td>0.000000</td>
<td>1.181727</td>
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Table A34: Cartesian coordinates in Angstroms (Å) for the $C_{2v}$ optimized geometry of Rb$^+$Ar$_4$ at the MP2/TZ level of theory.

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Table A35: Cartesian coordinates in Angstroms (Å) for the $T_d$ optimized geometry of Rb$^+$Ar$_4$ at the MP2/TZ level of theory.

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Table A36: Cartesian coordinates in Angstroms (Å) for the $C_{4v}$ optimized geometry of Rb$^+$Ar$_5$ at the MP2/TZ level of theory.

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<td>1.318763</td>
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Table A37: Cartesian coordinates in Angstroms (Å) for the $D_{3h}$ optimized geometry of Rb$^+$Ar$_5$ at the MP2/TZ level of theory.

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<tr>
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Table A38: Cartesian coordinates in Angstroms (Å) for the $C_{2v}$ optimized geometry of Rb$^+$Ar$_6$ at the MP2/TZ level of theory.

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<td>Ar</td>
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<tr>
<td>Ar</td>
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<td>0.295991</td>
<td>-3.065383</td>
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<tr>
<td>Ar</td>
<td>0.486342</td>
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Table A39: Cartesian coordinates in Angstroms (Å) for the $O_h$ optimized geometry of Rb$^+$Ar$_6$ at the MP2/TZ level of theory.

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<tr>
<td>Ar</td>
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<tr>
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<td>3.384149</td>
<td>0.000000</td>
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<tr>
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Table A40: Cartesian coordinates in Angstroms (Å) for the C$_{\infty v}$ optimized geometry of H$^-$Ar at the MP2/TZ level of theory.

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Table A41: Cartesian coordinates in Angstroms (Å) for the C$_{2v}$ optimized geometry of H$^-$Ar$_2$ at the MP2/TZ level of theory.

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Table A42: Cartesian coordinates in Angstroms (Å) for the D$_{\infty h}$ optimized geometry of H$^-$Ar$_2$ at the MP2/TZ level of theory.

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<td>1.000000</td>
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Table A43: Cartesian coordinates in Angstroms (Å) for the C\textsubscript{3v} optimized geometry of H\textsuperscript{−}Ar\textsubscript{3} at the MP2/TZ level of theory.

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Table A44: Cartesian coordinates in Angstroms (Å) for the C\textsubscript{2v} optimized geometry of H\textsuperscript{−}Ar\textsubscript{3} at the MP2/TZ level of theory.

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<td>−0.569047</td>
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Table A45: Cartesian coordinates in Angstroms (Å) for the C\textsubscript{2v} optimized geometry of H\textsuperscript{−}Ar\textsubscript{4} at the MP2/TZ level of theory.

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Table A46: Cartesian coordinates in Angstroms (Å) for the $T_d$ optimized geometry of $H^-\text{Ar}_4$ at the MP2/TZ level of theory.

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<td>-1.245833</td>
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Table A47: Cartesian coordinates in Angstroms (Å) for the $C_{4v}$ optimized geometry of $H^-\text{Ar}_5$ at the MP2/TZ level of theory.

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Table A48: Cartesian coordinates in Angstroms (Å) for the $D_{3h}$ optimized geometry of $H^-\text{Ar}_5$ at the MP2/TZ level of theory.

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Table A49: Cartesian coordinates in Angstroms (Å) for the $C_{2v}$ optimized geometry of $H^-\text{Ar}_6$ at the MP2/TZ level of theory.

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Table A50: Cartesian coordinates in Angstroms (Å) for the $O_h$ optimized geometry of $H^-\text{Ar}_6$ at the MP2/TZ level of theory.

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Table A51: Cartesian coordinates in Angstroms (Å) for the $C_{\infty v}$ optimized geometry of $F^-\text{Ar}$ at the MP2/TZ level of theory.

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Table A52: Cartesian coordinates in Angstroms (Å) for the $C_{2v}$ optimized geometry of $F^-\text{Ar}_2$ at the MP2/TZ level of theory.

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Table A53: Cartesian coordinates in Angstroms (Å) for the $D_{\infty h}$ optimized geometry of $F^-Ar_2$ at the MP2/TZ level of theory.

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Table A54: Cartesian coordinates in Angstroms (Å) for the $C_{3v}$ optimized geometry of $F^-Ar_3$ at the MP2/TZ level of theory.

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Table A55: Cartesian coordinates in Angstroms (Å) for the $C_{2v}$ optimized geometry of $F^-Ar_3$ at the MP2/TZ level of theory.

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Table A56: Cartesian coordinates in Angstroms (Å) for the $C_{2v}$ optimized geometry of $F^-\text{Ar}_4$ at the MP2/TZ level of theory.

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Table A57: Cartesian coordinates in Angstroms (Å) for the $T_d$ optimized geometry of $F^-\text{Ar}_4$ at the MP2/TZ level of theory.

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Table A58: Cartesian coordinates in Angstroms (Å) for the $C_{4v}$ optimized geometry of $F^-\text{Ar}_5$ at the MP2/TZ level of theory.

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Table A59: Cartesian coordinates in Angstroms (Å) for the $C_{4v}$ optimized geometry of $F^-\text{Ar}_5$ at the MP2/TZ level of theory.

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Table A60: Cartesian coordinates in Angstroms (Å) for the C$_{2v}$ optimized geometry of F$^-$Ar$_6$ at the MP2/TZ level of theory.

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Table A61: Cartesian coordinates in Angstroms (Å) for the O$_h$ optimized geometry of F$^-$Ar$_6$ at the MP2/TZ level of theory.

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Table A62: Cartesian coordinates in Angstroms (Å) for the $C_{\infty v}$ optimized geometry of $\text{Cl}^-\text{Ar}$ at the MP2/TZ level of theory.

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Table A63: Cartesian coordinates in Angstroms (Å) for the $C_{2v}$ optimized geometry of $\text{Cl}^-\text{Ar}_2$ at the MP2/TZ level of theory.

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Table A64: Cartesian coordinates in Angstroms (Å) for the $D_{\infty h}$ optimized geometry of $\text{Cl}^-\text{Ar}_2$ at the MP2/TZ level of theory.

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Table A65: Cartesian coordinates in Angstroms (Å) for the $C_{3v}$ optimized geometry of Cl$^-$.Ar$_3$ at the MP2/TZ level of theory.

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Table A66: Cartesian coordinates in Angstroms (Å) for the $C_{2v}$ optimized geometry of Cl$^-$.Ar$_3$ at the MP2/TZ level of theory.

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Table A67: Cartesian coordinates in Angstroms (Å) for the $C_{2v}$ optimized geometry of Cl$^-$.Ar$_4$ at the MP2/TZ level of theory.

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Table A68: Cartesian coordinates in Angstroms (Å) for the T$_d$ optimized geometry of Cl$^-$Ar$_4$ at the MP2/TZ level of theory.

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Table A69: Cartesian coordinates in Angstroms (Å) for the C$_{4v}$ optimized geometry of Cl$^-$Ar$_5$ at the MP2/TZ level of theory.

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Table A70: Cartesian coordinates in Angstroms (Å) for the D$_{3h}$ optimized geometry of Cl$^-$-Ar$_5$ at the MP2/TZ level of theory.

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Table A71: Cartesian coordinates in Angstroms (Å) for the C$_{2v}$ optimized geometry of Cl$^-$-Ar$_6$ at the MP2/TZ level of theory.

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Table A72: Cartesian coordinates in Angstroms (Å) for the $O_h$ optimized geometry of $\text{Cl}^-\text{Ar}_6$ at the MP2/TZ level of theory.

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Table A73: Cartesian coordinates in Angstroms (Å) for the $C_{\infty v}$ optimized geometry of $\text{Br}^-\text{Ar}$ at the MP2/TZ level of theory.

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Table A74: Cartesian coordinates in Angstroms (Å) for the $C_{2v}$ optimized geometry of $\text{Br}^-\text{Ar}_2$ at the MP2/TZ level of theory.

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Table A75: Cartesian coordinates in Angstroms (Å) for the $D_{\infty h}$ optimized geometry of $\text{Br}^-\text{Ar}_2$ at the MP2/TZ level of theory.

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Table A76: Cartesian coordinates in Angstroms (Å) for the $C_{3v}$ optimized geometry of $\text{Br}^-\text{Ar}_3$ at the MP2/TZ level of theory.

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<td>−1.276341</td>
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Table A77: Cartesian coordinates in Angstroms (Å) for the $C_{2v}$ optimized geometry of $\text{Br}^-\text{Ar}_3$ at the MP2/TZ level of theory.

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Table A78: Cartesian coordinates in Angstroms (Å) for the $C_{2v}$ optimized geometry of $\text{Br}^-\text{Ar}_4$ at the MP2/TZ level of theory.

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Table A79: Cartesian coordinates in Angstroms (Å) for the $T_d$ optimized geometry of $\text{Br}^-\text{Ar}_4$ at the MP2/TZ level of theory.

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Table A80: Cartesian coordinates in Angstroms (Å) for the C\textsubscript{4v} optimized geometry of Br\textsuperscript{−}-Ar\textsubscript{5} at the MP2/TZ level of theory.

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Table A81: Cartesian coordinates in Angstroms (Å) for the D\textsubscript{3h} optimized geometry of Br\textsuperscript{−}-Ar\textsubscript{5} at the MP2/TZ level of theory.

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Table A82: Cartesian coordinates in Angstroms (Å) for the C$_{2v}$ optimized geometry of Br$^-$-Ar$_6$ at the MP2/TZ level of theory.

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Table A83: Cartesian coordinates in Angstroms (Å) for the O$_h$ optimized geometry of Br$^-$-Ar$_6$ at the MP2/TZ level of theory.

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Table A84: Cartesian coordinates in Angstroms (Å) for the $C_{\infty v}$ optimized geometry of Li$^+$Ar at the MP2/QZ level of theory.

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Table A85: Cartesian coordinates in Angstroms (Å) for the $D_{\infty h}$ optimized geometry of Li$^+$Ar$_2$ at the MP2/QZ level of theory.

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Table A86: Cartesian coordinates in Angstroms (Å) for the $D_{3h}$ optimized geometry of Li$^+$Ar$_3$ at the MP2/QZ level of theory.

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Table A87: Cartesian coordinates in Angstroms (Å) for the T_d optimized geometry of Li^+Ar_4 at the MP2/QZ level of theory.

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Table A88: Cartesian coordinates in Angstroms (Å) for the C_{4v} optimized geometry of Li^+Ar_5 at the MP2/QZ level of theory.

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Table A89: Cartesian coordinates in Angstroms (Å) for the D$_{3h}$ optimized geometry of Li$^+$Ar$_5$ at the MP2/QZ level of theory.

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Table A90: Cartesian coordinates in Angstroms (Å) for the O$_h$ optimized geometry of Li$^+$Ar$_6$ at the MP2/QZ level of theory.

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Table A91: Cartesian coordinates in Angstroms (Å) for the $C_{\infty v}$ optimized geometry of Na$^+$Ar at the MP2/QZ level of theory.

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Table A92: Cartesian coordinates in Angstroms (Å) for the $D_{\infty h}$ optimized geometry of Na$^+$Ar$_2$ at the MP2/QZ level of theory.

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Table A93: Cartesian coordinates in Angstroms (Å) for the $C_{2v}$ optimized geometry of Na$^+$Ar$_2$ at the MP2/QZ level of theory.

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Table A94: Cartesian coordinates in Angstroms (Å) for the C$_{3v}$ optimized geometry
of Na$^+$Ar$_3$ at the MP2/QZ level of theory.

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Table A95: Cartesian coordinates in Angstroms (Å) for the C$_{2v}$ optimized geometry
of Na$^+$Ar$_3$ at the MP2/QZ level of theory.

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Table A96: Cartesian coordinates in Angstroms (Å) for the C$_{4v}$ optimized geometry
of Na$^+$Ar$_4$ at the MP2/QZ level of theory.

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Table A97: Cartesian coordinates in Angstroms (Å) for the T_d optimized geometry of Na^+Ar_4 at the MP2/QZ level of theory.

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Table A98: Cartesian coordinates in Angstroms (Å) for the C_{4v} optimized geometry of Na^+Ar_5 at the MP2/QZ level of theory.

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Table A99: Cartesian coordinates in Angstroms (Å) for the D$_{3h}$ optimized geometry of Na$^+$Ar$_5$ at the MP2/QZ level of theory.

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Table A100: Cartesian coordinates in Angstroms (Å) for the O$_h$ optimized geometry of Na$^+$Ar$_6$ at the MP2/QZ level of theory.

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<tr>
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<tr>
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Table A101: Cartesian coordinates in Angstroms (Å) for the $C_{\infty v}$ optimized geometry of $K^+\text{Ar}$ at the MP2/QZ level of theory.

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Table A102: Cartesian coordinates in Angstroms (Å) for the $C_{2v}$ optimized geometry of $K^+\text{Ar}_2$ at the MP2/QZ level of theory.

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Table A103: Cartesian coordinates in Angstroms (Å) for the $D_{\infty h}$ optimized geometry of $K^+\text{Ar}_2$ at the MP2/QZ level of theory.

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Table A104: Cartesian coordinates in Angstroms (Å) for the C\(_{3v}\) optimized geometry of K\(^+\)Ar\(_3\) at the MP2/QZ level of theory.

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Table A105: Cartesian coordinates in Angstroms (Å) for the C\(_{2v}\) optimized geometry of K\(^+\)Ar\(_3\) at the MP2/QZ level of theory.

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Table A106: Cartesian coordinates in Angstroms (Å) for the C\(_{2v}\) optimized geometry of K\(^+\)Ar\(_4\) at the MP2/QZ level of theory.

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Table A107: Cartesian coordinates in Angstroms (Å) for the $T_d$ optimized geometry of $K^+\text{Ar}_4$ at the MP2/QZ level of theory.

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Table A108: Cartesian coordinates in Angstroms (Å) for the $C_{4v}$ optimized geometry of $K^+\text{Ar}_5$ at the MP2/QZ level of theory.

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Table A109: Cartesian coordinates in Angstroms (Å) for the $D_{3h}$ optimized geometry of $K^+\text{Ar}_5$ at the MP2/QZ level of theory.

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Table A110: Cartesian coordinates in Angstroms (Å) for the $C_{2v}$ optimized geometry of $K^+\text{Ar}_6$ at the MP2/QZ level of theory.

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Table A111: Cartesian coordinates in Angstroms (Å) for the $O_h$ optimized geometry of $K^+\text{Ar}_6$ at the MP2/QZ level of theory.

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<td>0.000000</td>
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Table A112: Cartesian coordinates in Angstroms (Å) for the $C_{\infty v}$ optimized geometry of $\text{Rb}^+\text{Ar}$ at the MP2/QZ level of theory.

<table>
<thead>
<tr>
<th>Atom</th>
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<tbody>
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<td>0.019739</td>
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<tr>
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Table A113: Cartesian coordinates in Angstroms (Å) for the $C_{2v}$ optimized geometry of $\text{Rb}^+\text{Ar}_2$ at the MP2/QZ level of theory.

<table>
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Table A114: Cartesian coordinates in Angstroms (Å) for the $D_{\infty h}$ optimized geometry of Rb$^+$Ar$_2$ at the MP2/QZ level of theory.

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<tr>
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</tr>
<tr>
<td>Ar</td>
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<td>1.000000</td>
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<tr>
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Table A115: Cartesian coordinates in Angstroms (Å) for the $C_{3v}$ optimized geometry of Rb$^+$Ar$_3$ at the MP2/QZ level of theory.

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<td>-1.920959</td>
<td>-2.260006</td>
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<tr>
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<td>-1.920959</td>
<td>-2.260006</td>
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Table A116: Cartesian coordinates in Angstroms (Å) for the $C_{2v}$ optimized geometry of Rb$^+$Ar$_3$ at the MP2/QZ level of theory.

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<tr>
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<td>2.637401</td>
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<td>0.445101</td>
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<td>0.445101</td>
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Table A117: Cartesian coordinates in Angstroms (Å) for the $C_2v$ optimized geometry of Rb$^+$Ar$_4$ at the MP2/QZ level of theory.

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<tr>
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<td>Ar</td>
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<tr>
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Table A118: Cartesian coordinates in Angstroms (Å) for the $T_d$ optimized geometry of Rb$^+$Ar$_4$ at the MP2/QZ level of theory.

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<tbody>
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<tr>
<td>Ar</td>
<td>0.000000</td>
<td>0.000000</td>
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<tr>
<td>Ar</td>
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<td>2.751913</td>
<td>−1.123464</td>
</tr>
<tr>
<td>Ar</td>
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<td>−2.751913</td>
<td>−1.123464</td>
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Table A119: Cartesian coordinates in Angstroms (\(\text{\AA}\)) for the C\(_{4v}\) optimized geometry of Rb\(^+\)Ar\(_5\) at the MP2/QZ level of theory.

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<tr>
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<td>0.000000</td>
<td>0.410279</td>
</tr>
<tr>
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<td>0.410279</td>
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<tr>
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<tr>
<td>Ar</td>
<td>0.000000</td>
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<td>0.410279</td>
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</table>

Table A120: Cartesian coordinates in Angstroms (\(\text{\AA}\)) for the D\(_{3h}\) optimized geometry of Rb\(^+\)Ar\(_5\) at the MP2/QZ level of theory.

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<tbody>
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<tr>
<td>Ar</td>
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<tr>
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Table A121: Cartesian coordinates in Angstroms (Å) for the C$_{2v}$ optimized geometry of Rb$^+$Ar$_6$ at the MP2/QZ level of theory.

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<td>Ar</td>
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<tr>
<td>Ar</td>
<td>3.309792</td>
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<td>Ar</td>
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Table A122: Cartesian coordinates in Angstroms (Å) for the O$_h$ optimized geometry of Rb$^+$Ar$_6$ at the MP2/QZ level of theory.

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<th>Atom</th>
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</thead>
<tbody>
<tr>
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<td>0.000000</td>
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<tr>
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<td>0.000000</td>
<td>0.000000</td>
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</tr>
<tr>
<td>Ar</td>
<td>3.358967</td>
<td>0.000000</td>
<td>0.000000</td>
</tr>
<tr>
<td>Ar</td>
<td>0.000000</td>
<td>-3.358967</td>
<td>0.000000</td>
</tr>
<tr>
<td>Ar</td>
<td>0.000000</td>
<td>0.000000</td>
<td>-3.358967</td>
</tr>
<tr>
<td>Ar</td>
<td>-3.358967</td>
<td>0.000000</td>
<td>0.000000</td>
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<tr>
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Table A123: Cartesian coordinates in Angstroms (Å) for the $C_{\infty v}$ optimized geometry of H$^-\text{Ar}$ at the MP2/QZ level of theory.

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Table A124: Cartesian coordinates in Angstroms (Å) for the $C_{2v}$ optimized geometry of H$^-\text{Ar}_2$ at the MP2/QZ level of theory.

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Table A125: Cartesian coordinates in Angstroms (Å) for the $D_{\infty h}$ optimized geometry of H$^-\text{Ar}_2$ at the MP2/QZ level of theory.

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<tbody>
<tr>
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<td>1.000000</td>
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<tr>
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<td>1.000000</td>
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<tr>
<td>Ar</td>
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Table A126: Cartesian coordinates in Angstroms (Å) for the C$_{3v}$ optimized geometry of H−Ar$_3$ at the MP2/QZ level of theory.

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</table>

Table A127: Cartesian coordinates in Angstroms (Å) for the C$_{2v}$ optimized geometry of H−Ar$_3$ at the MP2/QZ level of theory.

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<td>−0.270455</td>
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Table A128: Cartesian coordinates in Angstroms (Å) for the C$_{2v}$ optimized geometry of H−Ar$_4$ at the MP2/QZ level of theory.

<table>
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<tr>
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<td>−0.577377</td>
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<tr>
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Table A129: Cartesian coordinates in Angstroms (Å) for the $T_d$ optimized geometry of $\text{H}^-\text{Ar}_4$ at the MP2/QZ level of theory.

<table>
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<td>Ar</td>
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Table A130: Cartesian coordinates in Angstroms (Å) for the $C_{4v}$ optimized geometry of $\text{H}^-\text{Ar}_5$ at the MP2/QZ level of theory.

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<td>Ar</td>
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<td>0.480840</td>
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Table A131: Cartesian coordinates in Angstroms (Å) for the D<sub>3h</sub> optimized geometry of H<sup>-</sup>Ar<sub>5</sub> at the MP2/QZ level of theory.

<table>
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<th>Atom</th>
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Table A132: Cartesian coordinates in Angstroms (Å) for the C<sub>2v</sub> optimized geometry of H<sup>-</sup>Ar<sub>6</sub> at the MP2/QZ level of theory.

<table>
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<th>Atom</th>
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<td>Ar</td>
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Table A133: Cartesian coordinates in Angstroms (Å) for the $O_h$ optimized geometry of $H^-\text{Ar}_6$ at the MP2/QZ level of theory.

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<td>0.000000</td>
</tr>
<tr>
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Table A134: Cartesian coordinates in Angstroms (Å) for the $C_{\infty v}$ optimized geometry of $F^-\text{Ar}$ at the MP2/QZ level of theory.

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Table A135: Cartesian coordinates in Angstroms (Å) for the $C_{2v}$ optimized geometry of $F^-\text{Ar}_2$ at the MP2/QZ level of theory.

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Table A136: Cartesian coordinates in Angstroms (Å) for the $D_{\infty h}$ optimized geometry of $F^-Ar_2$ at the MP2/QZ level of theory.

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Table A137: Cartesian coordinates in Angstroms (Å) for the $C_3v$ optimized geometry of $F^-Ar_3$ at the MP2/QZ level of theory.

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Table A138: Cartesian coordinates in Angstroms (Å) for the $C_{2v}$ optimized geometry of $F^-Ar_3$ at the MP2/QZ level of theory.

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Table A139: Cartesian coordinates in Angstroms (Å) for the $C_{2v}$ optimized geometry of $F^{-}\text{Ar}_4$ at the MP2/QZ level of theory.

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Table A140: Cartesian coordinates in Angstroms (Å) for the $T_d$ optimized geometry of $F^{-}\text{Ar}_4$ at the MP2/QZ level of theory.

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<td>1.771114</td>
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Table A141: Cartesian coordinates in Angstroms (Å) for the C$_{4v}$ optimized geometry of F$^{-}$Ar$_5$ at the MP2/QZ level of theory.

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Table A142: Cartesian coordinates in Angstroms (Å) for the C$_{4v}$ optimized geometry of F$^{-}$Ar$_5$ at the MP2/QZ level of theory.

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Table A143: Cartesian coordinates in Angstroms (Å) for the $C_{2v}$ optimized geometry of $F^-\text{Ar}_6$ at the MP2/QZ level of theory.

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Table A144: Cartesian coordinates in Angstroms (Å) for the $O_h$ optimized geometry of $F^-\text{Ar}_6$ at the MP2/QZ level of theory.

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Table A145: Cartesian coordinates in Angstroms (Å) for the $C_{\infty v}$ optimized geometry of Cl−Ar at the MP2/QZ level of theory.

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Table A146: Cartesian coordinates in Angstroms (Å) for the $C_{2v}$ optimized geometry of Cl−Ar$_2$ at the MP2/QZ level of theory.

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Table A147: Cartesian coordinates in Angstroms (Å) for the $D_{\infty h}$ optimized geometry of Cl−Ar$_2$ at the MP2/QZ level of theory.

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Table A148: Cartesian coordinates in Angstroms (Å) for the C₃ᵥ optimized geometry of Cl⁻Ar₃ at the MP2/QZ level of theory.

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Table A149: Cartesian coordinates in Angstroms (Å) for the C₂ᵥ optimized geometry of Cl⁻Ar₃ at the MP2/QZ level of theory.

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Table A150: Cartesian coordinates in Angstroms (Å) for the C₂ᵥ optimized geometry of Cl⁻Ar₄ at the MP2/QZ level of theory.

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Table A151: Cartesian coordinates in Angstroms (Å) for the T_d optimized geometry of Cl^-Ar_4 at the MP2/QZ level of theory.

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Table A152: Cartesian coordinates in Angstroms (Å) for the C_4v optimized geometry of Cl^-Ar_5 at the MP2/QZ level of theory.

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Table A153: Cartesian coordinates in Angstroms (Å) for the D_{3h} optimized geometry of Cl^{-}Ar_{5} at the MP2/QZ level of theory.

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Table A154: Cartesian coordinates in Angstroms (Å) for the C_{2v} optimized geometry of Cl^{-}Ar_{6} at the MP2/QZ level of theory.

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Table A155: Cartesian coordinates in Angstroms (Å) for the $O_h$ optimized geometry of Cl$^-$.Ar$_6$ at the MP2/QZ level of theory.

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<tr>
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Table A156: Cartesian coordinates in Angstroms (Å) for the $C_{\infty v}$ optimized geometry of Br$^-$.Ar at the MP2/QZ level of theory.

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Table A157: Cartesian coordinates in Angstroms (Å) for the $C_{2v}$ optimized geometry of Br$^-$.Ar$_2$ at the MP2/QZ level of theory.

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Table A158: Cartesian coordinates in Angstroms (\text{	extdegree}Å) for the D\textsubscript{\infty h} optimized geometry of \textit{Br}–\textit{Ar}\textsubscript{2} at the MP2/QZ level of theory.

<table>
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Table A159: Cartesian coordinates in Angstroms (\text{	extdegree}Å) for the C\textsubscript{3v} optimized geometry of \textit{Br}–\textit{Ar}\textsubscript{3} at the MP2/QZ level of theory.

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Table A160: Cartesian coordinates in Angstroms (\text{	extdegree}Å) for the C\textsubscript{2v} optimized geometry of \textit{Br}–\textit{Ar}\textsubscript{3} at the MP2/QZ level of theory.

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Table A161: Cartesian coordinates in Angstroms (Å) for the C$_{2v}$ optimized geometry of Br$^-$-Ar$_4$ at the MP2/QZ level of theory.

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Table A162: Cartesian coordinates in Angstroms (Å) for the T$_d$ optimized geometry of Br$^-$-Ar$_4$ at the MP2/QZ level of theory.

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Table A163: Cartesian coordinates in Angstroms (Å) for the C$_{4v}$ optimized geometry of Br$^{-}$Ar$_5$ at the MP2/QZ level of theory.

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Table A164: Cartesian coordinates in Angstroms (Å) for the D$_{3h}$ optimized geometry of Br$^{-}$Ar$_5$ at the MP2/QZ level of theory.

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Table A165: Cartesian coordinates in Angstroms (Å) for the $C_{2v}$ optimized geometry of Br$^-\text{Ar}_6$ at the MP2/QZ level of theory.

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Table A166: Cartesian coordinates in Angstroms (Å) for the $O_h$ optimized geometry of Br$^-\text{Ar}_6$ at the MP2/QZ level of theory.

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Figure A1: M⁺Ar₁ and X⁻Ar₁ interatomic distance scan for various ions. Shaded markers indicate CCSD(T) values, where empty markers indicate MP2 values. Black lines indicate QZ values, where blue lines indicate 5Z values.
Figure A2: Li$^+$Ar$_1$ interatomic distance scan at the MP2/XZ and CCSD(T)/XZ ($X = T, Q, \text{ and } 5$) level of theory.
Figure A3: $\text{Na}^+\text{Ar}_1$ interatomic distance scan at the MP2/$X$ and CCSD(T)/$X$ ($X = T, Q,$ and 5) level of theory.
Figure A4: \( \text{K}^+\text{Ar}_1 \) interatomic distance scan at the MP2/\( X \)Z and CCSD(T)/\( X \)Z (\( X = T, Q, \text{and} 5 \)) level of theory.
Figure A5: Rb⁺Ar₁ interatomic distance scan at the MP2/XZ and CCSD(T)/XZ (X = T, Q, and 5) level of theory.
Figure A6: H−Ar₁ interatomic distance scan at the MP2/XZ and CCSD(T)/XZ (X = T, Q, and 5) level of theory.
Figure A7: $F^-\text{Ar}_1$ interatomic distance scan at the MP2/$X$ and CCSD(T)/$X$ ($X = T, Q,$ and 5) level of theory.
Figure A8: Cl−Ar interatomic distance scan at the MP2/XZ and CCSD(T)/XZ (X = T, Q, and 5) level of theory.
Figure A9: Br⁻–Ar₁ interatomic distance scan at the MP2/XZ and CCSD(T)/XZ (X = T, Q, and 5) level of theory.
Figure A10: Li$^+$Ar$_2$ relaxed angular scan at the MP2/TZ and CCSD(T)/TZ ($X = T, Q, \text{and } 5$) level of theory.
Figure A11: Na$^+$Ar$_2$ relaxed angular scan at the MP2/XZ and CCSD(T)/XZ (X = T, Q, and 5) level of theory.
Figure A12: $\text{K}^+\text{Ar}_2$ relaxed angular scan at the MP2/$X$ and CCSD(T)/$X$ ($X = T, Q, \text{and} 5$) level of theory.
Figure A13: Rb$^+$Ar$_2$ relaxed angular scan at the MP2/XZ and CCSD(T)/XZ ($X = T$ and Q) level of theory.
Figure A14: H⁻Ar₂ relaxed angular scan at the MP2/XZ and CCSD(T)/XZ (X = T, Q, and 5) level of theory.
Figure A15: $\text{F}^-\text{Ar}_2$ relaxed angular scan at the MP2/$X$ and CCSD(T)/$X$ ($X = T, Q, \text{and } 5$) level of theory.
Figure A16: Cl−Ar2 relaxed angular scan at the MP2/XZ and CCSD(T)/XZ (X = T, Q, and 5) level of theory.
Figure A17: Br−Ar2 relaxed angular scan at the MP2/XZ and CCSD(T)/XZ ($X = T, Q,$ and 5) level of theory.
Figure A18: Br⁻Ar₂ relaxed angular scan at the MP2/TZ and CCSD(T)/TZ level of theory. Red indicates the use of a pseudopotential.
Figure A19: Br⁻Ar₂ relaxed angular scan at the MP2/QZ and CCSD(T)/QZ level of theory. Red indicates the use of a pseudopotential.
Figure A20: Br⁻ Ar₂ relaxed angular scan at the MP2/5Z and CCSD(T)/5Z level of theory. Red indicates the use of a pseudopotential.