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**Ab initio** studies of atomic properties and experimental behavior of element 119 and its lighter homologs

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Static dipole polarizabilities of element 119 and its singly charged cation are calculated, along with those of its lighter homologs, Cs and Fr. Relativity is treated within the 4–component Dirac-Coulomb formalism and electron correlation is included by the single reference coupled cluster approach with single, double, and perturbative triple excitations (CCSD(T)). Very good agreement with available experimental values is obtained for Cs, lending credence to the predictions for Fr and element 119. The atomic properties in group-1 are largely determined by the valence ns orbital, which experiences relativistic stabilization and contraction in the heavier elements. As a result, element 119 is predicted to have a relatively low polarizability (169.7 a.u.), comparable to that of Na. The adsorption enthalpy of element 119 on Teflon, which is important for possible future experimental studies of this element, is estimated as 17.6 kJ/mol, the lowest among the atoms considered here. © 2013 American Institute of Physics. [http://dx.doi.org/10.1063/1.4795433]

I. INTRODUCTION

The heaviest elements produced (but not yet approved by the IUPAC and IUPAP commissions) are elements 117 and 118, and the heaviest elements on which chemical experiments were performed are Cn (Z = 112) and Fl (Z = 114). Recently, a first attempt at production of element 119 was made at the GSI, Darmstadt, using the $^{50}$Ti+$^{249}$Bk nuclear reaction, which should yield the $^{295}$I19 and $^{296}$I19 isotopes in the 4n and 3n evaporation channels, respectively.

Theoretical investigations of electronic and chemical properties of superheavy elements are important in assigning these atoms their place in the periodic table and in gaining insight into the influence of relativistic effects on their chemical behavior. They can also be used in experimental research; for example, predictions of adsorption enthalpies ($\Delta H_{ads}$) of various surfaces can assist in characterizing and separating new elements produced in accelerators. To be reliable, theoretical predictions of atomic and chemical properties should be based on benchmark quality calculations, which treat relativity and electron correlation at the highest possible level.

Element 119 was studied in a number of previous papers. The earliest Dirac-Slater and Dirac-Fock (DF) calculations are reported in Refs. 8–10, 14, and 15. More recently, the ionization potential (IP), excitation spectra, and electron affinity (EA) of element 119 were calculated using the combination of Dirac-Coulomb-Breit Hamiltonian with the state of the art intermediate Hamiltonian Fock space coupled cluster (IHFS) approach for treatment of correlation. 16, 17 The polarizability ($\alpha$) of element 119 was calculated using the Douglas-Kroll approximation combined with the coupled cluster method with single, double, and perturbative triple excitations (DK+CCSD(T)). 18, 19 Finally, we have recently published a relativistic 4-component density functional theory (4c-DFT) study of the properties of M$_2$ and MAu dimers, where M = K, Rb, Cs, Fr, and element 119. 20 There, molecular properties (dissociation energies) were used to make predictions of the sublimation enthalpy ($\Delta H_{sub}$) of element 119 and its $\Delta H_{ads}$ on gold, silver, and platinum surfaces. It was shown that element 119 has the highest $\Delta H_{sub}$ and the lowest $\Delta H_{ads}$ of the group-1 elements considered there, due to the dramatic relativistic stabilization and contraction of its 8s orbital. In addition to the molecular calculations, we also examined trends in the atomic properties of group-1 elements. All the properties under consideration, such as IPs, EAs, polarizabilities, electronegativities, and atomic radii exhibit a trend reversal at Cs, caused by the relativistic effects experienced by the valence ns electrons of the heavier atoms in the group.

Here we present relativistic benchmark calculations of the static dipole polarizability of element 119 and its singly charged cation, together with its lighter homologs, Fr and Cs. The polarizability of Cs was determined to a very high precision from the time-of-flight of laser cooled and launched cesium atoms travelling through an electric field. 21 This value gives us a possibility of an assessment of the accuracy of our calculations and the reliability of the predictions for Fr and element 119. In addition, we estimate the $\Delta H_{ads}$ of element 119 on a Teflon surface. Following the eventual discovery of suitable isotopes of element 119, its volatility might be studied using some advanced chromatography (vacuum) techniques that can cope with the extremely short lifetime of this element. To guarantee the transport of element 119 through Teflon capillaries from the target chamber to the chemistry setup, it is important to know its $\Delta H_{ads}$ on Teflon.
II. METHOD AND COMPUTATIONAL DETAILS

A. Polarizabilities

Static dipole polarizabilities were obtained using the finite field approach, with atomic energies calculated for the free atoms and in the presence of a uniform electric field acting in the z direction, $F_z$. The energy of the atom in the presence of an electric field is given by

$$E(F_z) = E(0) + F_z \frac{\partial E(F_z)}{\partial F_z} \bigg|_{F_z=0} + \frac{1}{2} F_z^2 \frac{\partial^2 E(F_z)}{\partial^2 F_z} \bigg|_{F_z=0} + \cdots \quad (1)$$

The first term in this equation is the ground state energy of the atom in the absence of the electric field, the second term contains the dipole moment, which vanishes for atoms, and $\alpha$ appears in the third term,

$$\alpha = -2 \frac{\partial E(F_z)}{\partial F_z}. \quad (2)$$

Atomic energy calculations were performed for $F_z = 0, 0.0005,$ and $0.0010$ a.u., and the polarizabilities were obtained by numerical differentiation. Good linearity of the energy shift with respect to $F_z^2$ was observed.

The energy calculations were performed in the framework of the 4c Dirac-Coulomb Hamiltonian,

$$H_{DC} = \sum_i h_D(i) + \sum_{i<j} 1/r_{ij} \quad (3)$$

Here, $h_D$ is the one-electron Dirac Hamiltonian,

$$h_D(i) = c\sum a_i \cdot p_i + c^2 \beta_i + V_{nuc}(i), \quad (4)$$

where $\alpha$ and $\beta$ are the four-dimensional Dirac matrices. The nuclear potential takes into account the finite size of the nucleus, modeled by the Gaussian charge distribution.

The lowest-order relativistic correction to the two-electron term in the DC Hamiltonian (Eq. (3)) can be provided by the Gaunt operator, $-e^2(\alpha \cdot \alpha)/r_{ij}$. In our recent paper, we have made an estimate of the contribution of the Gaunt correction to the polarizabilities of group-2 elements and their singly and doubly charged ions. For all the systems studied there, including element 120, the Gaunt contribution to the calculated polarizabilities was quite small, between $-0.5$ and $+0.2$ a.u.; we thus neglect this term in our present work.

Correlation was included by the open-shell single reference relativistic CCSD(T) method. In order to analyse the contribution of electron correlation to the calculated polarizabilities, we also present results obtained using the Dirac-Hartree-Fock (DHF), second order Moller-Plesset perturbation theory (MP2), and single reference RCCSD methods.

Group-1 elements have one valence electron in the $ns$ shell, and thus we can also perform the energy calculations using the relativistic FSCC method, described in detail in Refs. 27 and 28. Thus, we are able to compare the performance of different CC schemes for treatment of polarizabilities. In the FSCC calculations, the closed-shell $M^+$ cations were used as reference states, and the model space $P$ consisted of the $ns$ valence orbital ($n = 6$ for Cs, $n = 7$ for Fr, and $n = 8$ for element 119).

Faegri’s dual family basis sets of uncontracted Gaussian-type orbitals were used for Cs and Fr. This type of basis set is not available for element 119; we therefore used a basis set constructed from Faegri’s basis set for element 118. The basis sets of the three atoms were augmented by adding diffuse and higher angular momentum functions until the calculated polarizabilities converged. The final basis sets were 26$s23p16d8f4g$ for Cs, 26$s23p18d13f6g2h$ for Fr, and 29$s26p20d15f6g2h$ for element 119. Virtual orbitals with energies above 50 a.u. were omitted, and 27, 41, and 51 electrons were correlated for Cs, Fr, and element 119, respectively. All the energy calculations were carried out using the DIRAC08 computational program package.

B. Adsorption on inert surfaces

For the calculation of adsorption energies, $E(x)$, of group-1 elements on Teflon, the following model of the van der Waals ad-atom-slab interaction was used,

$$E(x) = -\frac{3}{16} \left(\frac{\varepsilon - 1}{\varepsilon + 2}\right) \frac{\alpha_{at}}{\left(\frac{1}{\varepsilon_{slab}} + \frac{1}{\varepsilon}\right)x^3}, \quad (5)$$

where $\varepsilon_{slab}$ and $\varepsilon$ are the IP and the dielectric constant of the surface material (for Teflon, $\varepsilon_{slab} = 10.12$ eV and $\varepsilon = 2.04$), $\alpha_{at}$ and $\alpha$ are the IP and the polarizability of the ad-atom, and $x$ is the ad-atom-surface separation distance, approximated by the van der Waals radius ($R_{vdW}$) of the adsorbed atom. The $R_{vdW}$ of Fr and element 119 were obtained via a correlation between the known semiempirical $R_{vdW}$ in group 1 (Ref. 34) and the radius of the maximal charge density ($R_{max}$) of the valence $ns$ atomic orbitals.

The calculated $E(x) \approx -\Delta H_{ads}$ (for $P, V = \text{const}$) of a given element can be used to predict its relative yield at the end of an inert transport capillary or a column, taking into account the half-life $T_{1/2}$ of the studied isotope and the parameters of the capillary/column. The following equation is used:

$$\frac{N}{N_0} = \exp\left(-\frac{2}{T_{1/2}}\right) t_R. \quad (6)$$

Here $N_0$ is the number of particles (atoms) entering the column, $N$ is the number of particles exiting the column, and $t_R$ is the retention time in the column. The latter is given by the following equation,

$$t_R = \frac{z_A \alpha_c u_m}{Q} \exp\left(-\frac{\Delta H_{ads}}{k_B T_c}\right), \quad (7)$$

where $z_A$ is the mean coordinate of the adsorption zone, $\alpha_c$ is the column surface area per unit length, $Q$ is the volume flow rate, $u_m$ is the mean velocity of two-dimensional gas molecules; $\tau_0$ is the elementary adsorption sojourn time, $k_B$ is Boltzmann constant, and $T_c$ is the temperature of the column.
TABLE I. Calculated static dipole polarizabilities of Cs, Fr, and element 119 and their singly charged cations (a.u.).

<table>
<thead>
<tr>
<th></th>
<th>HF</th>
<th>MP2</th>
<th>FSCCSD</th>
<th>RCCSD</th>
<th>RCCSD(T)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cs</td>
<td>668.9</td>
<td>266.4</td>
<td>402.9</td>
<td>436.7</td>
<td>399.0</td>
</tr>
<tr>
<td>Cs+</td>
<td>15.6</td>
<td>15.5</td>
<td>15.5</td>
<td>15.5</td>
<td>15.5</td>
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<tr>
<td>Fr</td>
<td>526.1</td>
<td>182.6</td>
<td>316.2</td>
<td>342.4</td>
<td>311.5</td>
</tr>
<tr>
<td>Fr+</td>
<td>20.1</td>
<td>20.1</td>
<td>20.1</td>
<td>20.1</td>
<td>20.1</td>
</tr>
<tr>
<td>119</td>
<td>231.3</td>
<td>132.1</td>
<td>170.7</td>
<td>177.7</td>
<td>169.7</td>
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<tr>
<td>119+</td>
<td>32.8</td>
<td>30.8</td>
<td>31.6</td>
<td>31.6</td>
<td></td>
</tr>
</tbody>
</table>

III. RESULTS AND DISCUSSION

A. Polarizabilities

Table I contains polarizabilities of Cs, Fr, and element 119 and their singly charged cations, obtained using different correlation schemes. As the results show, DHF significantly overestimates the polarizabilities of the neutral atoms, while the MP2 correction gives a rather large error in the opposite direction (compared to the RCCSD(T) results). The contribution of triple excitations is of importance, as can be seen from comparing the RCCSD and RCCSD(T) values, lowering the calculated polarizabilities by 5%–10%. The FSCCSD method, however, reproduces well the RCCSD(T) values without explicit treatment of triple excitations. Close agreement of the FSCCSD and the RCCSD(T) results has been observed before, e.g., for the spectroscopic constants of the I2 and the I2+ molecules,

The RCCSD(T) results, which provide a more complete description of the triple excitations, are taken as the final recommended values. The effect of correlation on the calculated polarizabilities of the cations is negligible, due to the large energy gap between the highest occupied and lowest unoccupied orbitals.

Table II contains the recommended RCCSD(T) polarizabilities, compared to the most recent calculated and experimental values. Our value for Cs is in very good agreement with the experiment, as well as with the values obtained in previous publications using the relativistic single double excitation all-order approximation (R-SD) method and those obtained using the DK+CCSD(T) method in Ref. 19. Earlier DK+CCSD(T) investigations of Lim et al. seem to overestimate the polarizability of Cs compared to the experiment. This discrepancy was shown in Ref. 19 to arise both from the limited size of the basis set and from the insufficient degree of the polynomial fit used to obtain $\alpha$ from the point charge calculations.

The polarizability of Fr is yet to be measured; we thus compare our results with the other theoretical results. Our value is in good agreement with the most recent high quality ab initio investigations. The two previous calculations of $\alpha$ of element 119 are the 2003 and 1999 DK+CCSD(T) investigations of Lim et al. Both are in good agreement with our RCCSD(T) result. The remarkable agreement of the result from Ref. 18 with our number might be coincidental, as for the lighter elements larger discrepancies are observed.

The recommended atomic properties of group-1 elements are summarized in Table III: experimental values are used where available, IHFSSC results for the EA of Fr and EA and IP of element 119, and present calculations for the polarizabilities of Fr and element 119. Static atomic polarizability is linked to the atomic size, which in turn may be approximated by the cube of the radius of the maximal charge density of the valence orbital ($ns$ orbital in the case of group-1 elements studied here), $[R_{\text{max}}(ns)]^3$. For the neutral atoms, $\alpha$ increases from Na to Cs and then decreases towards element 119 (Fig. 1(a)), which can be explained by the strong relativistic contraction of the $ns$ orbital in the heavier elements. The polarizability of element 119 (169.7 a.u.) is thus similar to that of Na (162.7 ± 1.2 a.u.). Indeed, the nonrelativistic CCSD(T) value for the polarizability of element 119 calculated here is 646 a.u., the highest in the group, which highlights the importance of relativistic effects. The IPs and EAs decrease from Na to Cs and then increase again towards element 119. Thus, all the atomic properties considered here exhibit a distinct trend reversal at Cs, caused by the relativistic effects on the valence $ns$ orbital in the heavier homologues (as was also demonstrated in Ref. 20).

TABLE II. Static dipole polarizabilities of Cs, Fr, and element 119 and their cations (a.u.), compared to experiment for Cs and to other theoretical results.

<table>
<thead>
<tr>
<th></th>
<th>Method</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cs</td>
<td>RCCSD(T)</td>
<td>Present work</td>
</tr>
<tr>
<td>399.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>401.5</td>
<td>R-SDa</td>
<td>37</td>
</tr>
<tr>
<td>399.9</td>
<td>R-SDa</td>
<td>38</td>
</tr>
<tr>
<td>396.0</td>
<td>DK+CCSD(T)b</td>
<td>19</td>
</tr>
<tr>
<td>430</td>
<td>DK+CCSD(T)b+SOc</td>
<td>18</td>
</tr>
<tr>
<td>401.0 ± 0.6</td>
<td>Experimental</td>
<td>21</td>
</tr>
<tr>
<td>Cs+</td>
<td>RCCSD(T)</td>
<td>Present work</td>
</tr>
<tr>
<td>15.5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>15.8</td>
<td>RRPAc</td>
<td>37</td>
</tr>
<tr>
<td>15.0</td>
<td>DK+CCSD(T)b</td>
<td>39</td>
</tr>
<tr>
<td>15.8</td>
<td>DK+CCSD(T)b+SOc</td>
<td>40</td>
</tr>
<tr>
<td>Fr</td>
<td>RCCSD(T)</td>
<td>Present work</td>
</tr>
<tr>
<td>311.5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>313.7</td>
<td>R-SDa</td>
<td>41</td>
</tr>
<tr>
<td>315.1</td>
<td>R-SDa</td>
<td>37</td>
</tr>
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<td>315.2</td>
<td>DK+CCSD(T)b</td>
<td>19</td>
</tr>
<tr>
<td>318</td>
<td>DK+CCSD(T)b+SOc</td>
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<tr>
<td>Fr+</td>
<td>RCCSD(T)</td>
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</tr>
<tr>
<td>20.1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>20.4</td>
<td>RRPAc</td>
<td>37</td>
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<tr>
<td>19.2</td>
<td>DK+CCSD(T)b</td>
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</tr>
<tr>
<td>20.4</td>
<td>DK+CCSD(T)b+SOc</td>
<td>40</td>
</tr>
<tr>
<td>119</td>
<td>RCCSD(T)</td>
<td>Present work</td>
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<tr>
<td>169.7</td>
<td></td>
<td></td>
</tr>
<tr>
<td>166.0</td>
<td>DK+CCSD(T)b</td>
<td>19</td>
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<td>169</td>
<td>DK+CCSD(T)b+SOc</td>
<td>18</td>
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<tr>
<td>119+</td>
<td>RCCSD(T)</td>
<td>Present work</td>
</tr>
<tr>
<td>31.6</td>
<td></td>
<td></td>
</tr>
<tr>
<td>32.0</td>
<td>DK+CCSD(T)b+SOc</td>
<td>40</td>
</tr>
</tbody>
</table>

aRelativistic single double excitation all-order approximation.  
bdDouglas-Kroll combined with CCSD(T).  
ccSpin-orbit contributions calculated on the DHF level.  
rdRelativistic random-phase approximation (RRPA).

...
### TABLE III. IP, EAs (eV), and $\alpha$ (a.u.) of group-1 elements.

<table>
<thead>
<tr>
<th></th>
<th>IP$^a$</th>
<th>EA$^b$</th>
<th>$\alpha$$^c$</th>
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<tbody>
<tr>
<td>Na</td>
<td>5.139</td>
<td>0.547</td>
<td>162.7</td>
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<tr>
<td>K</td>
<td>4.341</td>
<td>0.501</td>
<td>290.6</td>
</tr>
<tr>
<td>Rb</td>
<td>4.177</td>
<td>0.486</td>
<td>318.8</td>
</tr>
<tr>
<td>Cs</td>
<td>3.894</td>
<td>0.472</td>
<td>401.0$^d$</td>
</tr>
<tr>
<td>Fr</td>
<td>4.073</td>
<td>0.491$^e$</td>
<td>311.5$^e$</td>
</tr>
<tr>
<td>119</td>
<td>4.783$^g$</td>
<td>0.663$^e$</td>
<td>169.7$^f$</td>
</tr>
</tbody>
</table>

$^a$Experimental, Ref. 43.  
$^b$Experimental, Ref. 44.  
$^c$Experimental, Ref. 42.  
$^d$Experimental, Ref. 21.  
$^e$Theoretical, IHFSCC, Ref. 16.  
$^f$Theoretical, present RCCSD(T) results.  
$^g$Theoretical, IHFSCC, Ref. 17.

In the case of the cations, a different trend in polarizabilities is observed (Fig. 1(b)), defined by the outer $(n-1)p_{3/2}$ orbital, which expands in the group with an increase in the atomic number. Thus, $119^+$ has the highest polarizability of group-1 cations.

### B. Adsorption on Teflon

The $R_{vdW}$ of group-1 elements are presented in Table IV and in Fig. 2(a). The trend in $R_{vdW}$ follows that of $R_{max}$ of the valence $ns$ orbitals, with a maximum at Cs and a subsequent decrease towards element 119, caused by the relativistic contraction of the valence $ns$ orbital in the heavier elements.

The $-\Delta H_{ads}$ of group-1 elements calculated using Eq. (5) are also shown in Table IV. They decrease with increasing atomic number (Fig. 2(b)), so that the predicted $-\Delta H_{ads}$ of element 119 is the lowest among the atoms considered here, as is the case with its $-\Delta H_{ads}$ on noble metals calculated in Ref. 20. The low value of 17.6 kJ/mol indicates that this atom should be easily transported through the Teflon capillaries to the chemistry set up. Using the obtained $-\Delta H_{ads}$ of element 119 and Eqs. (6) and (7) we have calculated the relative yield of the $^{295}119$ isotope with $T_{1/2} = 1$ s at the end of an open Teflon column or a capillary with an inner diameter of 2 mm, length of 1 m, and $Q = 1$ l/min, at room temperature, as 78%. The low adsorption enthalpy of element 119 means that in this case the yield at the end of the column or capillary is not determined by its volatility, but rather by the lifetime of a given isotope with respect to the transport time.
IV. SUMMARY AND CONCLUSION

We have calculated the polarizabilities of the neutral atom and the singly charged cation of element 119 and its lighter homologs Cs and Fr, using the combination of the 4c DC Hamiltonian and the CCSD(T) approach. Excellent agreement with experiment was obtained for Cs; a similar accuracy is expected for our predictions for Fr and element 119. For these systems we find that the performance of the FSCC method is similar to that of the CCSD(T) approach, and exceeds the quality of the CCSD calculations, as it captures the majority of the triple excitations contribution.

The atomic properties of the group-1 atoms are largely determined by their valence $\text{ns}$ orbital, which experiences strong relativistic stabilization and contraction in the heavier elements. Thus, the polarizabilities increase in the group from Na to Cs and decrease towards element 119, having $\Delta$ of 169.7 a.u., similar to that of Na. Other atomic properties, i.e., IPs, EAs, and $R_{\text{opt}}$ also experience a trend reversal at Cs.

Based on the atomic properties of element 119, its $-\Delta H_{\text{ads}}$ on Teflon is estimated as 17.6 kJ/mol, the lowest among the group-1 elements considered here and is low enough to allow an easy transport of this atom through the Teflon capillaries to the chemistry set up.

ACKNOWLEDGMENTS

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