

Ionization potential and electron affinity of element 119: calculations in optimized Gaussian basis set

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This paper presents the optimized basis set of Gaussian functions for relativistic calculations of chemical properties of the superheavy element with nuclear charge $Z = 119$. The obtained basis set was used to calculate ionization potential and electron affinity of element 119 within the framework of the single-reference coupled cluster method and the Fock-space coupled cluster method.

Keywords: superheavy elements, element 119, basis optimization, relativistic effects, correlation effects, quantum electrodynamics corrections.

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Introduction

The discovery and study of new chemical elements has long been one of the most important areas of physical research [1]. At present, the heaviest synthesized superheavy element (SHE) is oganesson (Og, $Z = 118$) [2], which is the last member of the seventh period of the periodic table. The next element is eka-francium, which is also known as ununennium (Uue, $Z = 119$) and has not been synthesized yet. An attempt at synthesis of element 119 (E119) was made at the Helmholtz Centre for Heavy Ion Research in Darmstadt (GSI) [3]. An experiment has also been conducted for several years at the Institute of Physical and Chemical Research in Japan (RIKEN) [4]. Experiments on synthesis of eka-francium are planned to be carried out at the Joint Institute for Nuclear Research (JINR) [5] and the Zhejiang Institute of Modern Physics (IMP) [6].

Research interest in superheavy elements stems largely from the desire to determine the limits of applicability of the periodic law, which states that elements of the same group (homologues) should have similar properties. However, it is not uncommon for certain properties of superheavy elements to differ significantly from the corresponding characteristics of their lighter homologues. For example, it was established in [7] that oganesson has a positive electron affinity, which distinguishes it radically from other noble gases. The difference in electronic structure between SHEs and their lighter homologues is associated, on the one hand, with an increase in the number of core electrons and the core size and, on the other hand, with a more profound influence of

relativistic effects induced by an increase in the nuclear charge [8].

The ionization potential (IP), electron affinity (EA), and polarizability of E119 were calculated in [9–16]. Calculations for the chemical properties of compounds E119H, E119F, and E119Cl were performed in [13,17,18]. Most of these calculations relied on basis sets obtained using the GCDF (generator coordinate Dirac–Fock) method [19,20] and its refined polynomial version (p -GCDF) [21]. These basis sets are tailored for calculations by the Dirac–Fock method and, consequently, may turn out to be suboptimal when applied in calculations with correlation effects taken into account. In the present study, the basis set of Gaussian functions for eka-francium obtained by the p -GCDF method in [18] is optimized. The optimized basis set and the coupled cluster method are used to refine the ionization potential and electron affinity values of E119.

Theoretical methods

The DIRAC [22,23] and EXP-T [24,25] packages were used to calculate the ionization potential and electron affinity of eka-francium. The relativistic Fock-space coupled cluster (FS-CC) method [26] was used to introduce the effects of electron correlation in preliminary calculations. This approach involves constructing an effective Hamiltonian in a model space defined by the chosen valence one-electron functions. In our calculation, sectors $0h0p$, $0h1p$, and $0h2p$ of the Fock space correspond to configurations $[\text{Rn}]5f^{14}6d^{10}7s^27p^6$ (cation), $[\text{Rn}]5f^{14}6d^{10}7s^27p^68s^1$ (neutral atom), and

[Rn] $5f^{14}6d^{10}7s^27p^68s^2$ (anion), respectively. The generalized relativistic core potential (GRECP) method [27,28], which allowed us to exclude 110 core electrons from analysis, was used to optimize the basis set of Gaussian functions within the FS-CC approach.

According to the results of preliminary FS-CC calculations, the ground states of a neutral atom of E119 and its cation and anion may be described by the single-reference method. Therefore, the final calculations of ionization potential and electron affinity were performed within the single-reference coupled cluster approach with account for single, double, and perturbative triple excitations (CCSD(T)). The four-component relativistic Dirac–Coulomb (DC) Hamiltonian was used:

$$H_{DC} = \Lambda^+ \left[\sum_{i=1}^N h_i^D + \sum_{\substack{i=2, \\ j<i}}^N \frac{1}{r_{ij}} \right] \Lambda^+, \quad (1)$$

where h^D is the one-electron Dirac Hamiltonian that includes interaction with a nucleus with its charge density characterized by a Gaussian distribution [29], N is the number of electrons, r_{ij} is the distance between electrons i and j , and Λ^+ is the direct product of one-electron projectors by the positive spectrum of Dirac–Fock operator h^{DF} .

We did also calculate additional corrections to the ionization potential and electron affinity that incorporate the contributions of the Gaunt interaction and quantum electrodynamic effects. Gaunt interaction operator

$$V_{ij}^G = -\frac{(\boldsymbol{\alpha}_i \cdot \boldsymbol{\alpha}_j)}{r_{ij}} \quad (2)$$

was introduced into calculations at the stage of constructing the one-electron basis set by the Dirac–Fock method with the use of the two-component relativistic mean-field Hamiltonian (X2Cmmf) [30]. The X2Cmmf Hamiltonian is constructed in such a way that it reproduces the positive spectrum of the Dirac–Fock equation [31–32]. Quantum electrodynamic corrections were calculated by the Dirac–Fock (DF) and configuration interaction (CI) methods in the Dirac–Fock–Sturm (DFS) orbital basis. A detailed description of these methods is provided in [9,33,34].

Calculation details

Basis optimization

The basis presented in [18] was chosen to be the initial approximation. This set of Gaussians was obtained by the p -GCDF [21] method and has a relatively small number of functions ($34s31p23d18f$), which may affect the accuracy of determination of calculated quantities. The

optimization procedure consists in adding new functions to the existing set in a sequential manner. The parameters of these new functions are selected based on the variation of IP and EA in the FS-CC calculation. As was already noted, the GRECP pseudopotential was used in the process of basis set optimization. All orbitals occupied in the reference determinant (Fermi vacuum) and virtual orbitals below 50 a.u. were included in the correlation calculation performed by the FS-CC method with account for single and double excitations (FS-CCSD). The $8s$ orbital was included in the active space.

The optimization procedure is similar to those detailed in [35,36]. Let us denote the basis chosen to be the initial approximation as χ_0 , add s -function $\gamma_1^s(\alpha)$ with parameter α to basis set χ_0 , and perform the FS-CCSD calculation for the $\alpha \in [0.0001, 1000]$ parameter range. Basis function $\gamma_1^s(\alpha_1)$ providing the largest contribution to the IP and EA change relative to the values of atomic properties without this function is included in the basis set: $\chi_0 + \gamma_1^s(\alpha_1) \equiv \chi_1^s$. The procedure is repeated until the change in IP and EA with added function $(k+1)$ relative to the calculation in basis χ_k^s becomes smaller than a preset value (0.001 eV). The new basis containing k added optimized s -functions is denoted as

$$\chi_0 + \sum_{m=1}^k \gamma^s(\alpha_m) \equiv \chi^s. \quad (3)$$

The above procedure is then repeated for p -functions (with the parameters of basis functions from the previous step remaining unchanged). The basis with k optimized s -functions and k' optimized p -functions is denoted as

$$\chi^s + \sum_{m=1}^{k'} \gamma_m^p(\alpha_m) \equiv \chi^p. \quad (4)$$

We then add functions with higher orbital quantum numbers up to $l = 6$ in a similar fashion, forming the resulting basis set χ^i . Table 1 lists the changes in IP and EA values and the cation (E_{00}), neutral atom (E_{01}), and anion (E_{02}) energies obtained after adding a new λ -function, $\lambda = s, \dots, i$, to the basis already optimized for quantum number λ . It is evident that, in accordance with what was written above, the changes in IP and EA do not exceed 0.001 eV. The most profound change in the absolute values of energy (approximately 0.007 eV) is observed when additional function i is introduced. The parameters of optimized basis exponents are presented in the Appendix.

Final calculation

As was already noted, the final results for IP and EA were obtained using the four-component DC Hamiltonian. Single, double, and perturbative triple excitations (SR-CCSD(T)) were taken into account in calculations by the single-reference coupled cluster method. The correlation of

Table 1. Variation of the values of ionization potential (IP); electron affinity (EA); and cation (E_{00}), neutral atom (E_{01}), and anion (E_{02}) energies induced by the addition of function with orbital momentum λ ($\lambda = s, \dots, i$) to set χ^λ . The values are expressed in eV

λ	ΔIP	ΔEA	ΔE_{00}	ΔE_{01}	ΔE_{02}
<i>s</i>	0.00007	0.00007	0.00010	0.00011	0.00013
<i>p</i>	0.00001	0.00002	0.00014	0.00015	0.00015
<i>d</i>	0.00011	0.00017	0.00085	0.00096	0.00110
<i>f</i>	0.00004	0.00013	0.00060	0.00062	0.00064
<i>g</i>	0.00023	0.00104	0.00342	0.00345	0.00346
<i>h</i>	0.00018	0.00011	0.00272	0.00289	0.00296
<i>i</i>	0.00025	0.00034	0.00704	0.00718	0.00725

Table 2. Comparison of IP and EA calculated with non-optimized (χ_0) and optimized (χ^i) basis sets using the SR-CCSD(T) method (eV)

Basis	IP	EA
χ_0	4.649	0.415
χ^i	4.795	0.674

109 electrons was factored in, and the active space consisted of virtual orbitals with energies no higher than 1000 a.u.

Calculations by the Fock-space coupled cluster method with account for single and double excitations (FS-CCSD) were performed in order to compare the optimized basis with the basis from [20] that was used in [10,12,13]. Virtual orbitals with energies below 100 a.u. were included in the correlation calculation. The active space consisted of the 8s orbital. The correlation of 78 and 50 electrons was taken into account in IP and EA calculations, respectively. These calculation parameters match the corresponding ones from [10,12].

Calculation results

Using the χ_0 basis taken from [18] and our optimized χ^i basis set, we calculated the IP and EA of element 119 by the SR-CCSD(T) method. The results are listed in Table 2. It can be seen that the procedure of basis optimization alters the IP and EA of element 119 significantly: both values increase approximately by 0.15 eV. This is especially noticeable in the case of electron affinity, which changes by about 60% of its value calculated with the non-optimized basis.

Table 3 presents the IP and EA calculated by the FS-CCSD method with the GRECP pseudopotential for each basis set χ^λ (see the previous section). These data allow one to track the evolution of the ionization potential and electron affinity in the course of optimization and reveal

Table 3. Ionization potential (IP) and electron affinity (EA) calculated with χ^λ basis sets (eV). Designation χ^λ ($\lambda = s, \dots, i$) refers to a basis set obtained after optimizing the functions of each symmetry with $l \leq \lambda$. χ_0 is the initial approximation basis set. Calculations were performed using the FS-CCSD method and the GRECP pseudopotential

Basis	IP	EA
χ_0	4.6602	0.4919
χ^s	4.6706	0.5674
χ^p	4.6703	0.6376
χ^d	4.6705	0.6388
χ^f	4.7590	0.6943
χ^g	4.7744	0.7033
χ^h	4.7783	0.7061
χ^i	4.7796	0.7068

that the optimization of functions with almost every value of angular momentum λ leads to an increase in the ionization potential and electron affinity relative to the values obtained in the basis where the λ symmetry functions were not optimized. The optimization of *s*-, *p*-, and *f*-functions produces a significant contribution to the IP and EA variation, indicating clearly that the initial χ_0 basis is suboptimal for characterizing the atomic properties of E119. The values of IP and EA calculated in the fully optimized basis with the pseudopotential were 4.7796 and 0.7068 eV, respectively.

Table 4 lists the contributions to the ionization potential and electron affinity from the Gaunt interaction, self-energy (SE), and Uehling (Ue) and Wichmann–Kroll (WK) potentials calculated by the Fock-space coupled cluster method (FS-CCSD), the Dirac–Fock (DF) method, and the configuration interaction method (CI-DFS). The overall contribution from quantum electrodynamic corrections (QED) is also indicated. Owing to the lack of additivity, the sum of the SE, Ue, and WK contributions does not match the overall QED contribution. The overall QED contribution was calculated by adding the model operator to the Hamiltonian. The obtained multielectron wave functions with the overall QED contribution factored in were used to calculate individual contributions as average values of the corresponding operators. The final values of IP and EA were adjusted to include the overall contribution from quantum electrodynamic corrections.

The contribution of the Breit interaction to the ionization potential was calculated in [12,14,15] and is estimated at 24–35 cm^{−1}, which corresponds to the magnitude of the Gaunt contribution calculated here (31 cm^{−1}). The contribution of QED effects to IP and EA was also estimated in [9,11–15,37–42]. Comparing the overall QED correction (101 cm^{−1}) to the ionization potential with the results obtained in [9,12–15,39–42], one finds that the values reported earlier deviate significantly from it, varying

Table 4. Additional contributions to the ionization potential (IP) and electron affinity (EA) from the Gaunt interaction, self-energy (SE), and Uehling (Ue) and Wichmann–Kroll (WK) potentials. The overall contribution from quantum electrodynamic corrections is denoted as QED. The contribution of the Gaunt interaction was calculated using the FS-CCSD method, and the remaining contributions were calculated within the DF and CI-DFS approaches. The values are expressed in eV

Characteristic	Contribution	DF	CI-DFS	FS-CCSD
IP	Gaunt			−0.0038
	SE	−0.0236	−0.0231	
	Ue	0.0118	0.0117	
	WK	−0.0009	−0.0009	
	SE+Ue+WK	−0.0127	−0.0123	
	QED	−0.0123	−0.0126	
EA	Gaunt			−0.0005
	SE	−0.0057	−0.0067	
	Ue	0.0030	0.0034	
	WK	−0.0002	< 0.0000	
	SE+Ue+WK	−0.0029	−0.0034	
	QED	−0.0028	−0.0032	

from 67 [14] to 152 cm^{−1} [40]. The contribution of quantum electrodynamic effects to the electron affinity was calculated in [11] to be 100 cm^{−1}, which is also quite far from the value obtained in the present study (26 cm^{−1}).

The IP and EA values obtained here and the corresponding results from [9–13,15] are listed in Table 5. The Dirac–Coulomb–Breit Hamiltonian was used in all these studies. It follows from Table 5 that the results of our FS-CCSD calculations of ionization potential and electron affinity are in reasonable agreement with the corresponding values calculated by the same method in [10,12]. Slight discrepancies between the obtained values are attributable to the use of different basis sets, the lack of a QED correction to the electron affinity in [10], the use of different values of the QED contribution to the ionization potential in the present study and in [12], and the inclusion of the retarded part of the Breit interaction in calculations in [10,12]. The other calculation parameters in the present study and in [10,12] match. The key advantage of our basis set is that the electron correlation was taken into account in the process of optimization of Gaussians. In addition, our optimized basis (41s37p25d22f4g4h2i) contains fewer *g*-, *h*-, and *i*-functions than the basis from [20] (36s32p24d22f10g7h6i), which makes it suitable for application in molecular calculations.

The results reported in [13] are of particular note. The ionization potential obtained in this study is consistent (within 0.01 eV) with the results of other studies. However, the electron affinity presented in [13] differs from the values reported elsewhere approximately by 0.2 eV, which is about

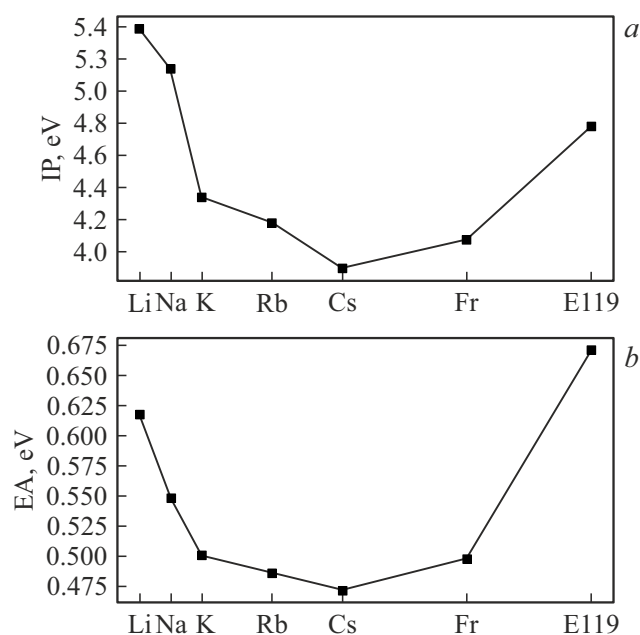
Table 5. Comparison of IP and EA of element 119 obtained here with the results of other studies (eV). The values determined in the present study are separated by a horizontal line

Method	IP	EA
SR-CCSD	4.717	0.595
SR-CCSD(T)	4.779	0.671
FS-CCSD	4.769	0.707
CI-DFS+MBPT [9]	4.768	0.674
FS-CCSD [10]		0.7171
IHFS-CCSD [11]		0.64870
FS-CCSD [12]	4.7829	
FS-CCSD [13]	4.7838	0.4850
CPM [15]	4.7779	

30–40% of the EA value. The authors of [10] and [13] used the same basis set taken from [20], the same software package [43], and the same virtual spaces. A noticeable difference between [10] and [13] lies in the number of correlated electrons (50 and 28, respectively), but such a large EA difference cannot be attributed to this factor. Thus, it remains unclear why the EA value given in [13] differs so significantly from the data reported elsewhere.

Our best results presented here are the values calculated using the SR-CCSD(T) method: 4.779(10) eV for the ionization potential and 0.671(4) eV for the electron affinity. To estimate the error, we performed two scalar-relativistic calculations using the GRECP pseudopotential in the CFOUR [44] package with the optimized basis and the same basis with 6g4h3i-functions added to it and calculated the difference between the obtained ionization potential and electron affinity values. Thus, errors were estimated as the contribution of high harmonics in the scalar-relativistic calculation. The values calculated by the SR-CCSD(T) method differ slightly from those obtained within FS-CCSD. The application of the SR-CCSD(T) approach has a particularly noticeable effect on the electron affinity, which becomes closer to the values from [9]. Owing to the single-reference approach, we may also estimate the perturbative contribution of triple excitations: it is close to 0.06 eV for IP and 0.08 eV for EA.

The comparison of obtained data with the characteristics of lighter SHE homologues is a rather important part of the study of properties of superheavy elements. Figure 5 shows the dependences of IP and EA of alkali metals on their nuclear charge. The IP and EA values decrease through to cesium and start increasing beyond this point. This behavior is associated with relativistic effects that arise due to contraction of the *s* and *p* shells. In the non-relativistic limit, these dependencies decrease monotonically (see, e.g., [9]).



(a) Ionization potentials for elements of the first group of the periodic table. Experimentally obtained IP values for Li–Fr were taken from [45–52]. (b) Electron affinity for elements of the first group. Experimentally measured EA values for Li–Cs were reported in [53–58], and the EA for Fr was obtained theoretically in [9].

Conclusion

The basis set of Gaussians for the superheavy element with nuclear charge $Z = 119$ was optimized. The obtained basis was used to calculate the ionization potential and electron affinity of this element. Calculations were performed in the DIRAC [22,23] and EXP-T [24,25] packages by the SR-CC method with account for single, double, and perturbative triple excitations and by the FS-CC method with account for single and double excitations. The contributions of the Gaunt interaction and QED effects for IP and EA were also calculated.

The addition of new basis functions has produced a significant contribution to the IP and EA values. The absolute changes of these parameters were on the order of 0.15 eV. The calculated ionization potential and electron affinity values are in reasonable agreement with the results of earlier studies. The optimized set of Gaussians provides a fine description of three E119 states: a neutral atom, a cation, and an anion. In addition, our basis set is significantly smaller than those presented in other studies. Taken together, these factors make the resulting set suitable for calculation not only of the atomic properties, but also of molecules containing element 119.

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Conflict of interest

The authors declare that they have no conflict of interest.

Appendix: basis for element 119

Parameters of Gaussians for each orbital quantum number λ (a.u.). The values without an asterisk (*) correspond to the exponent parameters taken from [18]. The values with an asterisk correspond to the exponent parameters optimized in the FS-CCSD calculation

№	λ						
	s	p	d	f	g	h	i
1	2.92537106e+11	6.42563106e+07	6.94530747e+05	3.12565925e+04	9.841600e-01*	1.028690e+00*	8.248500e-01*
2	2.45266474e+09	2.26791996e+07	2.05423290e+05	1.55041364e+04	6.743300e-01*	7.038800e-01*	2.803300e-01*
3	6.10698516e+08	8.47630044e+06	6.76728912e+04	7.85584415e+03	4.495500e-01*	2.415500e-01*	
4	1.66834382e+08	3.34276066e+06	2.45977608e+04	4.05799545e+03	1.969100e-01*	1.319300e-01*	
5	4.97353022e+07	1.38604772e+06	9.77239832e+03	2.13273926e+03			
6	1.60921834e+07	6.02113947e+05	4.20378443e+03	1.13816590e+03			
7	5.62065186e+06	2.73061476e+05	1.93964546e+03	6.15529780e+02			
8	2.10780484e+06	1.28818151e+05	9.50946000e+02	3.36668400e+02			
9	8.44105249e+05	6.29915378e+04	4.90738240e+02	1.85865810e+02			
10	3.59034179e+05	3.18148239e+04	2.64066570e+02	1.03365260e+02			
11	1.61323810e+05	1.65376059e+04	1.46776120e+02	5.77912100e+01			
12	7.61614365e+04	8.81587038e+03	8.34804400e+01	3.24186600e+01			
13	3.75747637e+04	4.80242771e+03	4.81294000e+01	1.82099500e+01			
14	1.92678102e+04	2.66387106e+03	2.78638700e+01	1.02220200e+01			
15	1.02139547e+04	1.49925645e+03	1.60467300e+01	5.72286000e+00			
16	5.56713119e+03	8.53105330e+02	9.10657000e+00	3.18913000e+00			
17	3.10309764e+03	4.89042980e+02	5.04493000e+00	1.76542000e+00			
18	1.75928572e+03	2.81425010e+02	2.70269000e+00	9.68890000e-01			
19	1.00903159e+03	1.61995620e+02	1.38704000e+00	5.40450000e-01*			
20	5.82305770e+02	9.29442300e+01	9.56490000e-01*	3.60350000e-01*			
21	3.36299220e+02	5.29631400e+01	6.75520000e-01	1.71730000e-01*			
22	1.93321230e+02	2.98683300e+01	3.09280000e-01	7.01600000e-02*			
23	1.10017730e+02	1.66106900e+01	1.31870000e-01				
24	6.16489600e+01	9.07732000e+00	5.18700000e-02				
25	3.38313400e+01	4.85707000e+00	1.96100000e-02*				
26	1.80839600e+01	2.53566000e+00					
27	9.36482000e+00	1.28695000e+00					
28	4.67291000e+00	9.60000000e-01*					
29	3.31527000e+00*	6.32760000e-01					
30	2.23464000e+00	4.17530000e-01*					
31	1.48976000e+00*	3.00320000e-01					
32	1.01862000e+00	1.37100000e-01					
33	4.40200000e-01	9.00000000e-02*					
34	2.79070000e-01*	5.99900000e-02					
35	1.79380000e-01	4.00000000e-02*					
36	1.03000000e-01*	1.48700000e-02*					
37	6.85500000e-02						
38	2.44400000e-02						
39	1.03300000e-02*						
40	6.27000000e-03*						
41	3.03000000e-03*						

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