Relativistic coupled-cluster calculations of spectroscopic and chemical properties for element 120

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ABSTRACT

The coupled cluster calculations taking into account relativistic effects to study spectroscopic and chemical properties of element 120 (E120) are performed. A generalized relativistic effective core potential for the 10 explicitly treated electrons of E120 atom was generated to perform molecular calculations. Similar calculations for Ba are also done and they are in a good agreement with the experimental data. Dissociation energies of diatomic X–H and X–Au molecules, where X = E120, Ba, are calculated; for E120 they are found to be 1.5—2 times smaller than those for Ba.

1. Introduction

At present all the relatively long-lived superheavy elements (SHEs) up to the seventh period of the Periodic table with the exception of element 118 were synthesized in FLNR JINR (see [1,2] and references) and their synthesis was mainly confirmed in LBNL [3] and GSI [4]. A new challenge for nuclear physics is the synthesis of the elements of the eight period.

According to its position in the Periodic table, element 120 (E120) is supposed to be the s element and homologue of Ba and Ra. The earlier obtained ground state configuration of E120 at the Dirac–Fock level, $7s^2 7p^6 8s^2$, is confirmed in the recent calculation [5] using a correlation potential method. A relativistic stabilization of the valence s orbital [6,7] leads, in general, to a higher excitation energies from this shell and, as a consequence, to a weakening the bond strengths in its chemical compounds. Therefore, E120 can resemble the noble gas rather than the alkaline earth element. Provided that E120 is synthesized, its properties can be investigated experimentally by the gas-phase chromatography method. Such a scheme was successfully employed in FLNR JINR [8] and GSI [4] for E112 and E114 where gold served as an adsorbent. Theoretical calculations are required for planning similar experiments with E120 on the gold surface.

In the absence of any experimental data, some accurate ab initio calculations of the properties of simple E120 compounds performed with an explicit treatment of correlation effects can be used to calibrate DFT functionals to study more complicated systems containing E120. As shown in [9], most of the popular DFT functionals failed to describe the adsorption of copernicium and mercury at the gold clusters simulating surface, therefore, a careful calibration of the DFT functionals is important to model the adsorption of E120 on the gold surface. To our knowledge ab initio calculations with explicit treatment of correlation effects were performed only for E120^{2+}, E120$^+$, E120 [5,10] and E120H$^+$ molecule [11] till now. There are also relativistic density functional calculations [12] for the E120$_2$ and E120Au molecules compared to their lighter analogues. In this work we have performed accurate coupled-cluster calculations of excitation energies of the E120 atom and its cation, E120$^+$, as well as of spectroscopic properties of the E120H and E120Au molecules compared to the analogous systems with Ba, for which some experimental data are available.

2. Computational method

To study properties of E120, the generalized relativistic effective core potential (GRECP) method [13] was employed. For the relativistic correlation treatment, the fully-relativistic Fock-space coupled cluster code with single and double cluster amplitudes (FS-RCCSD) [14,7] was applied. To evaluate corrections on the enlargement of the basis set and higher cluster amplitudes, the CFOUR [15] and MRCC [16,17] codes were used.

2.1. GRECP generation and atomic calculations

The GRECP for E120 was generated in the framework of the present work. To check the performance of the GRECP method for such a heavy element, relativistic correlation calculations on the E120 atom and its cations were carried out. We used four-component calculations with Dirac–Coulomb–Breit (DCB) Hamiltonian and Fermi nuclear charge distribution ($A = 304$) as the reference study. This Hamiltonian takes into account a great bulk of the relativistic effects including the relativistic corrections to the

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Coulomb interaction between electrons. The 1-5s, 2-5p, 3-5d, and 4-5f shells were frozen from the E120^{2+} ground state calculation. The 28 electrons (occupying the 6spd, 7spd, 8sp shells) were correlated in the [12,14,14,13,12,11] basis set of 6-17$s_{1/2}$, 6-19$p_{1/2}$, 6-19$p_{3/2}$, ..., 6-16$h_{11/2}$ numerical spinors localized in the same radial space region as the 6spd, 7spd, 8sp spinors. The correlations were taken into account with the help of the FS-RCCSD method. The closed-shell ground state of E120^{2+} was a reference state and the Fock-space scheme was

$$E120^{2+} \rightarrow E120^{+} \rightarrow E120, \tag{1}$$

with the electrons added to the 8$s_{1/2}$, 8$p_{1/2}$, 8$p_{3/2}$, 7$d_{3/2}$, and 7$d_{5/2}$ spinors (the relativistic configurations corresponding to the nonrelativitic 8p^2, 7d^2, and 8$p^1 7d^1$ ones were excluded from the model space).

The leading configurations and terms for the lowest-lying states of the E120 atom and its cations are presented in the first and second columns of Table 1. The results of the semiempirically-fitted CI/MBPT calculations with Dirac–Coulomb Hamiltonian [5,10] are compared with our FS-RCCSD results in the fourth and fifth columns. They are in a reasonable agreement. The absolute errors due to a decrease in the number of the correlated electrons, neglect of a finite nuclear size or Breit interactions are listed in the last four columns. One can see that a finite nuclear size should be taken into account, whereas the correlations with the 6spd electrons and Breit interactions can be neglected for the accuracy within 2 kcal/mol ≈700 cm^{-1} for one-electron excitations.

We have generated the GRECP for only 10 explicitly treated electrons of E120 (i.e., with the 7spd, 8sp, 6f, 5g GRECP components) following the scheme [18] just to reduce unnecessary computational efforts at the stage of the correlation molecular calculations (see below); a similar GRECP version was generated earlier for Ba [19]. The results for the 10 correlated electrons (occupying the 7spd, 8sp shells) in the [9,11,11,9,8,7] basis set of 7-15$s_{1/2}$, 7-17$p_{1/2}$, 7-17$p_{3/2}$, ... 6-12$h_{11/2}$ numerical spinors localized in the same radial space region as the 7spd, 8sp spinors are presented in Table 2. The transition energies from the DCB/FS-RCCSD calculations with a Fermi nuclear model and the absolute

errors of their reproducing in the GRECP calculations are tabulated in the third and fourth columns.

The calculations with different approximations to the "full" GRECP operator are considered in the last four columns. If one neglects the difference between the outercore (7sp) and valence (8sp) GRECP components, two extreme GRECP versions can be derived with the conventional semi-local RECP operator: only valence or only outercore GRECP components acting on both valence and outercore electrons. These cases are referred to as the valence or core GRECP versions, respectively [13]. One can see that the full and valence GRECP versions are suitable for the accuracy of 2 kcal/mol ≈ 700 cm^{-1} whereas the core GRECP version is not. It should be noted that the errors of neglecting the innercore correlations with the 6spd shells and the errors of the GRECP approximation are partly compensating each other, thus, it additionally justifies our choice of the 10-electron GRECP for the present molecular calculations.

The scalar-relativistic (SR) calculations, i.e., without a spin–orbit (SO) part of the valence GRECP operator, are presented in the seventh column. The SO contributions are large and should be taken into account. The scalar-relativistic SCF calculations followed by the FS-RCCSD calculations with the SO part of the valence GRECP operator are presented in the last column. These errors are comparable with the errors of the valence GRECP calculations in the fifth column. It should be emphasized that the GRECP calculations presented in the 4–6th columns were carried out with the SO part at both SCF and FS-RCCSD stages. The computational versions used in the last two columns (the SR SCF calculation followed by the scalar-relativistic or fully-relativistic coupled cluster study) are also used in the molecular correlation calculations discussed below.

To compare with the E120 transition energies, the corresponding experimental data for Ba from Ref. [20] are listed in Table 1. One can see that the barium excitation energies are smaller in general. It also indicates that E120 will possibly be more inert in general than Ba.

2.2. Molecular calculations

In two-component molecular relativistic calculations and a high-level correlation treatment only relatively small basis sets can be used for the diatomics like E120Au. At the same time, rather

Table 1

Transition energies (TE) from DCB/FS-RCCSD calculations of the lowest-lying states of the E120 atom and its cations for 28 correlated electrons with Fermi nuclear model and Breit interactions taken into account. The absolute errors of reproducing the TE in different versions of the four-component calculations. The experimental transition energies from Ref. [20] for the lowest-lying states of the Ba atom and its cations are given for comparison. All values are in cm^{-1}.

Leading conf.[a]	Term	Ba Ref. [20]	TE Ref. [5,10]	TE	Abs. errors			Point nucl.	Without Breit
Number of corr.el.				28	20	10		28	28
$s^1_{1/2}$	($J = 1/2$)	→							
$p^1_{1/2}$	($J = 1/2$)	20262	24851	24551	55	−372		1299	−51
$d^1_{3/2}$	($J = 3/2$)	4874		25355	43	−151		1714	135
$d^1_{5/2}$	($J = 5/2$)	5675		27529	20	−481		1661	152
$p^1_{3/2}$	($J = 3/2$)	21952	38057	37643	23	−401		1632	62
Ba^{2+}/E120^{2+}	($J = 0$)	80686	89931	89601	36	−620		1592	77
$s^2_{1/2}$	($J = 0$)	→							
$s^1_{1/2}p^1_{1/2}$	($J = 0$)	12266	16061	15328	58	−290		975	−45
$s^1_{1/2}p^1_{1/2}$	($J = 1$)	12637	17968	17382	50	−290		1015	−30
$s^1_{1/2}d^1_{3/2}$	($J = 1$)	9034	23066	22337	30	−145		1242	101
$s^1_{1/2}d^1_{3/2}$	($J = 2$)	9216	23231	22494	24	−249		1212	101
$s^1_{1/2}d^1_{5/2}$	($J = 3$)	9597	23827	23377	12	−418		1186	108
$s^1_{1/2}p^1_{3/2}$	($J = 2$)	13515	25457	25308	26	−264		1186	42
$s^1_{1/2}d^1_{5/2}$	($J = 2$)	11395	27477	27652	15	−401		1347	100
$s^1_{1/2}p^1_{3/2}$	($J = 1$)	18060	27685	28304	3	−422		1024	39
$s^1_{1/2}$	($J = 1/2$)	42035	47296[b]	47633	11	−458		906	40

[a] Main quantum numbers are 8 for s, 8 for p, 7 for d in the case of E120 and 6 for s, 6 for p, 5 for d in the case of Ba.

[b] The first ionization potential for the E120 atom was calculated as 44 118 cm^{-1} by the DC/FS-RCCSD method in paper [11].

Table 2

Transition energies (TE) from DCB/FS-RCCSD calculations of the lowest-lying states of the E120 atom and its cations for the 10 correlated electrons with the Fermi nuclear model and Breit interaction are taken into account. The absolute errors of reproducing the TE with different versions of the GRECP calculations. All values are in cm^{-1}.

Leading conf.	Term	TE	GRECP abs. errors				
		DCB	Full	Val.	Core	Val. SR	Val. SR-SCF SO-RCC
$8s^1_{1/2}$	$(J = 1/2)$	→					
$8p^1_{1/2}$	$(J = 1/2)$	24142	247	306	−2761	9255	393
$7d^1_{3/2}$	$(J = 3/2)$	25241	399	436	−1766	1316	358
$7d^1_{5/2}$	$(J = 5/2)$	27071	389	447	−1765	−514	447
$8p^1_{3/2}$	$(J = 3/2)$	37194	326	392	−1937	−3797	257
$E120^{2+}$	$(J = 0)$	88907	446	554	−1701	−739	417
$8s^2_{1/2}$	$(J = 0)$	→					
$8s^1_{1/2}8p^1_{1/2}$	$(J = 0)$	15012	266	310	−2354	6960	−100
$8s^1_{1/2}8p^1_{1/2}$	$(J = 1)$	17064	251	295	−2341	4908	−171
$8s^1_{1/2}7d^1_{3/2}$	$(J = 1)$	22207	366	401	−1632	585	316
$8s^1_{1/2}7d^1_{3/2}$	$(J = 2)$	22259	387	428	−1620	533	483
$8s^1_{1/2}7d^1_{5/2}$	$(J = 3)$	22968	386	436	−1617	−176	484
$8s^1_{1/2}8p^1_{3/2}$	$(J = 2)$	25009	253	297	−1842	−3037	384
$8s^1_{1/2}7d^1_{5/2}$	$(J = 2)$	27271	344	394	−1813	−262	291
$8s^1_{1/2}8p^1_{3/2}$	$(J = 1)$	27834	307	351	−1820	−1171	563
$8s^1_{1/2}$	$(J = 1/2)$	47120	333	385	−1661	−687	381

large basis sets can be employed in scalar-relativistic calculations of diatomic molecules. Therefore, the following scheme for the basis set generation was used in this work: (i) For each atom (E120, Ba and Au), a large set of primitive Gaussian functions capable of describing the wave-functions of the ground and excited states of the corresponding atoms was generated. These basis sets will be referred as LBas below. LBas (E120) and LBas (Ba) consist of $15s$-,$15p$-,$8d$-,$8f$-,$6g$-,$6h$-type functions, which shortly can be written as (15,15,8,8,6,6). (ii) Then a scalar relativistic CCSD calculation is performed with the large basis set for an atom and its compound (E120, E120–H, E120–Au, etc.). (iii) A generation of a compact basis set of the contracted Gaussian functions was performed in a manner similar to that employed for the generating atomic natural basis sets [21]: the atomic blocks from the density matrix calculated at the stage (ii) were diagonalized to yield atomic natural-like basis set. The functions with the largest occupation numbers were selected from these natural basis functions. The results obtained with the given basis set approximately reproduce those with the large basis set. Besides, the functions required for an accurate reproduction of the essentially different radial parts of the $7p_{1/2}$ and $7p_{3/2}$ spinors, as well as the $8p_{1/2}, 8p_{3/2}, 7d_{3/2},$ and $7d_{5/2}$ spinors, have also been included to the new basis set. These compact basis sets will be referred to as CBas.

Finally, the following scheme to evaluate ionization potentials and dissociation energies of molecules was employed: (i) Calculation using the two-component Fock-space coupled cluster method with single and double cluster amplitudes in the CBas basis set. (ii) Calculation of the corrections on the enlargement of the basis set and contribution of the triple cluster amplitudes by a scalar-relativistic coupled cluster method with single, double and non-iterative triple cluster amplitudes, CCSD (T), using LBas. (iii) Calculation of the corrections on the higher (iterative triple and non-iterative quadruple) cluster amplitudes by the scalar-relativistic coupled cluster method with single, double, triple and non-iterative quadruple cluster amplitudes, CCSDT (Q), using CBas.

The scheme described above was employed to calculate the potential curves of the diatomic molecules under consideration. These curves were then used to calculate the spectroscopic properties such as equilibrium internuclear distances, vibrational constants, etc.

3. Results and discussions

3.1. Ionization potentials

Some properties of E120, of which the first (IP1) and second (IP2) ionization potentials are examples, are considered here in comparison with the corresponding properties of Ba. As it was described above, the two-component FS-RCCSD method was used to calculate the main contributions to IP1 and IP2. These calculations were performed with the compact basis sets, CBas, consisting of $5s, 6p, 4d,$ and $3f$ functions for E120 and of $5s, 5p, 3d,$ and $3f$ for Ba. The computed values for E120 are IP1 = 47236 cm^{-1} and IP2 = 89061 cm^{-1}, while for Ba IP1 = 42340 cm^{-1} and IP2 = 80326 cm^{-1}. The contributions from the enlargement of the basis set up to $15s, 15p, 8d, 8f, 6g$ and $6h$ (15,15,8,8,6,6) functions and non-iterative triple cluster amplitudes for E120 are −462 cm^{-1} for IP1 and 31 cm^{-1} for IP2.[1] For Ba these values are −579 and −65 cm^{-1}. The contributions of higher cluster amplitudes estimated using the CCSDT (Q) method and (15,15,8,8,6) basis set (h functions were excluded) are negligible (less than 30 cm^{-1}). The final values of the ionization potentials for E120 and Ba are given in Table 4 together with the corresponding experimental values for Ba.

The self-energy and vacuum polarization QED corrections were calculated in [10,22] as about 100–200 cm^{-1} for the ionization potential. They are not considered in the present Letter because they have the same order as error of the current correlation calculation.

3.2. X–H dissociation energies, X = E120, Ba

In order to estimate the stability of compounds of E120 compared to those of Ba we have considered first the dissociation energies of the corresponding hydrides since the experimental data are available for BaH [23]. Another characteristics of SHEs often considered is a dissociation energy of its fluorides, X–F. However, the X–F bonding is not so illustrative qualitatively because almost all the elements (except light noble gases) are known to react in a

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[1] We have also included here the corrections arising when going from the Fock-space coupled clusters to the single-reference coupled clusters.

Table 3

The calculated dissociation energy of BaH and E120H using scalar-relativistic Hartree–Fock (HF) or FS-RCCSD levels of the theory in CBas basis set and CBas with excluded d-f-functions on Ba and E120 (CBasNoD).

Basis	CBas		CBasNoD	
Method	HF	FS-RCCSD	HF	FS-RCCSD
D_e(BaH), cm^{-1}	13 605	16 846	8634	11 699
D_e(E120H), cm^{-1}	2642	8117	61	6366

Table 4

The calculated properties of E120 in comparison with Ba: the first and second ionization potentials (IP1 and IP2), dissociation energies (D_e), equilibrium internuclear distances (R_e), harmonic frequency (w_e), vibrational anharmonicity ($w_e x_e$) of hydrides and aurides (X–Au). The relativistic DFT results of [12] are also presented for the comparison.

	E120-calc	Ba-calc	Ba-exp
IP1, cm^{-1}	47 046	41 932	42 035 [28]
IP2, cm^{-1}	89 286	80 442	80 686 [28]
D_e (X–H), cm^{-1}	8053	16 631	$\leqslant$16 308 [23]
R_e(X–H), Å	2.38	2.24	2.23 [24]
w_e(X–H), cm^{-1}	1070	1158	1168 [24]
$w_e x_e$(X–H), cm^{-1}	20.1	14.1	14.5 [24]
D_e (X–Au), cm^{-1}	14 537	22 909	–
	15 341 [12]	24 245 [12]	
R_e (X–Au), Å	3.03	2.91	–
	3.05 [12]	2.87 [12]	
w_e (X–Au), cm^{-1}	100	125	129 [23]
	97 [12]	145 [12]	
$w_e x_e$ (X–Au), cm^{-1}	0.13	0.16	0.18 [23]

fluorine atmosphere yielding rather stable fluorides. At the same time the dimer systems such as Ba_2, Hg_2, Xe_2, $E112_2$ are all the van der Waals systems with small dissociation energies. In contrast, the ground state of the XeH molecule is not observed in the gas phase, whereas BaH is obtained and characterized [24,25].

To calculate E120H and BaH, the scheme similar to that for the calculation of the ionization potentials was used. The compact basis sets for E120, Ba and H were [5,6,4,2], [5,5,3,2], and [4,3,1], respectively. The large basis sets for E120 and Ba were (15,15,8,8,6), i.e., without h-functions. The aug-cc-pvqz [26] basis set was used as a large basis set for H. To exclude the basis set superposition errors, the diatomic molecules and atoms were calculated in the same two-center basis, i.e., the counterpoise corrections [27] were used.

The dissociation energy of E120H calculated within FS-RCCSD using the CBas (E120) and CBas (H) basis sets is 8117 cm^{-1}, while the correction on the large basis and triple cluster amplitudes is -64 cm^{-1}. For BaH the former contribution is 16 846 cm^{-1}, while the correction is -215 cm^{-1}.

The final values for the dissociation energies and other calculated spectroscopic properties of E120H and BaH are given in Table 4. The equilibrium internuclear distance in BaH is by 0.14 Å shorter than that in E120H.[2]

It follows from Table 4 that the E120–H bond is significantly weaker than that in BaH. Partly it can be explained by the presence of lower-lying excited states in the case of Ba and its cation (see Table 1). A contribution of these states to the BaH chemical bond leads to its additional stabilization. In turn, the excited states in the case of E120 are lying significantly higher (see Table 2);

To check this viewpoint, two series of the FS-RCCSD calculations of the BaH and E120H dissociation energies were performed: (i) with d- and f- type basis functions included in the basis set (CBas); (ii) without d and f functions. The latter calculation prevents a par-

ticipation of the d orbitals of Ba and E120 in a chemical bonding of their hydrides. Note, however, that it is just a test calculation because the exclusion of d basis functions also prevents, e.g., the correlation of $5p$-electrons of Ba and $7p$-electrons of E120 into these states. The results are given in Table 3.

It follows from Table 3 that d functions (and higher harmonics) significantly contribute to the bonding of the monohydrides under consideration. At the FS-RCCSD level of the theory, this contribution is 5147 cm^{-1} to the Ba–H bond, while only 1751 cm^{-1} for E120H. These values confirm the qualitative discussion above based on the atomic transitions. However, even without the d basis functions, the BaH bond energy at the FS-RCCSD level is twice more than that in E120H. This observation is in a qualitative agreement with the fact that the states with the valence sp (p) configurations in E120 (E120$^+$) lie higher than the corresponding states in Ba (Ba$^+$). It should be noted that the bonding in E120H is in essence due to the correlation effects when the CBasNoD basis set is used.

3.3. X–Au dissociation energies, X = E120, Ba

As the first stage of modelling the interaction of E120 with the gold surface, the simplest comparative model, E120Au vs. BaAu, is considered here.

The 19-electron GRECP was used for Au. Thus, 29 electrons were treated in the correlation calculation. For E120Au, the relativistic two-component FS-RCCSD calculation in the Au [7,7,4,2] and E120 [5,5,2,1] basis sets gives the dissociation energy of 11 535 cm^{-1}. The correction on a larger basis set (15,15,8,8,7) for Au and [15,15,8,4] for E120) is 837 cm^{-1}, the contribution of non-iterative triple cluster amplitudes[3] is 2262 cm^{-1} and the correction on higher amplitudes (calculated as the difference between CCSDT (Q) and CCSD (T) energies in the compact Au [6,6,4,2,1] and E120 [6,5,2,1] basis sets) is less than 100 cm^{-1}. Similar calculations were performed for BaAu. The final calculated values are given in Table 4.

The equilibrium distance for BaAu is by 0.12 Å shorter than that in E120Au.

4. Conclusion

The properties of E120 and its compounds are considered in comparison with their Ba analogues. The monohydride and monoauride of E120 are found to be less stable than the corresponding analogues of the Ba compounds. Such a trend in decreasing the dissociation energies with E120 compared to lighter homologue is mainly due to a dramatic increase of the $s \rightarrow d$ excitation energy in E120 compared to Ba (it is the lowest-lying excitation for Ba), whereas the $s \rightarrow p$ excitation energy increase is not so large (it is the lowest-lying excitation for E120) because of strong relativistic stabilization of the s and $p_{1/2}$ shells and destabilization of d shells in the case of the superheavy elements. Nevertheless, E120 can be rather considered as a "typical" representative of the second group by its chemical properties.

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[2] Note that similar relation between internuclear distances takes place in E120H$^+$ and BaH$^+$ that is considered and discussed in [11].

[3] We have also included here the corrections arising when going from the Fock-space coupled clusters to the single-reference coupled clusters.

molecular calculations were performed at the Supercomputer "Lomonosov".

References

[1] Y. Oganessian, Eur. Phys. A 42 (3) (2009) 361.
[2] Y.T. Oganessian, F.S. Abdullin, P.D. Bailey, D.E. Benker, M.E. Bennett, S.N. Dmitriev, et al., Phys. Rev. Lett. 104 (2010) 142502.
[3] L. Stavsetra, K.E. Gregorich, J. Dvorak, P.A. Ellison, M.A. Garcia, et al., Phys. Rev. Lett. 103 (2009) 132502.
[4] J.M. Gates, C.E. Düllmann, M. Schädel, A. Yakushev, A. Türler, K. Eberhardt, et al., Phys. Rev. C 83 (2011) 054618.
[5] T.H. Dinh, V.A. Dzuba, V.V. Flambaum, J.S.M. Ginges, Phys. Rev. A 78 (2008) 054501.
[6] P. Schwerdtfeger, M. Seth, Relativistic effects of the superheavy elements, in: P. von Ragué Schleyer et al. (Eds.), Encyclopedia of Computational Chemistry, vol. 4, Wiley, New York, 1998, p. 2480.
[7] U. Kaldor, E. Eliav, A. Landau, Four-component relativistic coupled cluster – method and applications, in: K. Hirao, Y. Ishikawa (Eds.), Recent Advances in Relativistic Molecular Theory, World Scientific, Singapore, 2004, p. 283.
[8] R. Eichler, N.V. Aksenov, A.V. Belozerov, et al., Nature 447 (2007) 72.
[9] A. Zaitsevskii, A. Titov, Interaction of Copernicium with Gold: Assessment of Applicability of Simple Density Functional Theories, 2012. Available at: <http://arxiv.org/abs/1202.4723>.
[10] T.H. Dinh, V.A. Dzuba, V.V. Flambaum, J.S.M. Ginges, Phys. Rev. A 78 (2008) 022507.
[11] C. Thierfelder, P. Schwerdtfeger, A. Koers, A. Borschevsky, B. Fricke, Phys. Rev. A 80 (2009) 022501.
[12] V. Pershina, A. Borschevsky, J. Anton, J. Chem. Phys. 136 (13) (2012) 134317 (p. 10).
[13] N.S. Mosyagin, A.V. Zaitsevskii, A.V. Titov, Rev. Atomic Mol. Phys. 1 (1) (2010) 63.
[14] U. Kaldor, E. Eliav, A. Landau, RCCSD; Program Package for Calculation of Molecules by the Relativistic Fock-Space Coupled-Cluster Method.
[15] J.F. Stanton, J. Gauss, M.E. Harding, P.G. Szalay, et al., CFOUR; 2011, CFOUR: A Program Package for Performing High-level Quantum Chemical Calculations on Atoms and Molecules. Available at: <http://www.cfour.de>.
[16] M. Kállay, P.R. Surján, J. Chem. Phys. 115 (7) (2001) 2945, http://dx.doi.org/10.1063/1.1383290.
[17] M. Kállay, J. Gauss, P.G. Szalay, J. Chem. Phys. 119 (6) (2003) 2991, http://dx.doi.org/10.1063/1.1589003.
[18] N.S. Mosyagin, A.N. Petrov, A.V. Titov, I.I. Tupitsyn, Progr. Theor. Chem. Phys. B15 (2006) 229.
[19] M.G. Kozlov, A.V. Titov, N.S. Mosyagin, P.V. Souchko, Phys. Rev. A 56 (5) (1997) R3326.
[20] Y. Ralchenko, A. Kramida, J. Reader, NIST Atomic Spectra Database (ver. 4.1.0), National Institute of Standards and Technology, Gaithersburg, MD, 2011. Available at: <http://physics.nist.gov/asd>.
[21] J. Almlöf, P.R. Taylor, J. Chem. Phys. 86 (7) (1987) 4070.
[22] C. Thierfelder, P. Schwerdtfeger, Phys. Rev. A 82 (2010) 062503.
[23] K.P. Huber, G. Herzberg, Constants of Diatomic Molecules, Van Nostrand-Reinhold, New York, 1979.
[24] L.B. Knight, W.C. Easley, W. Weltner, J. Chem. Phys. 54 (1) (1971) 322.
[25] K.A. Walker, H.G. Hedderich, P.F. Bernath, Mol. Phys. 78 (3) (1993) 577.
[26] T.H. Dunning Jr., J. Chem. Phys. 90 (2) (1989) 1007.
[27] S.F. Boys, F. Bernardi, Mol. Phys. 19 (4) (1970) 553.
[28] C.E. Moore, Atomic Energy Levels, vol. 1–3, Circ. No. 467, Natl. Bur. Stand. (US), Washington, 1958. Available at: <http://www.nist.gov/srd/nsrds.cfm>.