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Atomic radii, Ionization Energies, and Polarizabilities of Heavy Atoms Au, At, and Ts and their Ions: Unveiling Relativistic Effects with ZORA and Schrödinger Hamiltonians

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Abstract :

This study investigates some of the atomic properties of heavy elements, namely Gold (Au), Astatine (At), and Tennessine (Ts), along with their ions (±1). Employing ZORA and Schrödinger Hamiltonians at the Hartree-Fock (HF) level, the analysis covers radii, ionization energies, and polarizabilities. The study explores the influence of basis set size using dyall.npz (n= D, T, Q). Results indicate good agreement of polarizabilities with experimental values in the relativistic case employing the dyall.4zp basis set. Radii also exhibit excellent agreement with other theoretical values in the relativistic scenario using dyall.npz basis sets. Noteworthy is the observation of $p_{3/2}$ spinor expansion in Astatine and Tennessine atoms due to relativistic effects, suggesting potential impacts on bond lengths in relevant molecules. Furthermore, this work introduces first-time calculations for properties related to astatine and tennessine ions, enriching the understanding of these heavy elements.

Key words : gold, astatine, tennessine, radii, ionization energy, polarizability , ZORA Hamiltonian.

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أنصاف الأقطار الذرية وكمونات التأين والأستقطابيات للذرات الثقيلة الذهب والأستاتين والتينيسين وأيوناتها: دراسة الأفعال النسبوية باستخدام هاملتونيي شرودنجر وZORA

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الملخص

تتناول هذه الدراسة بعض الخصائص الذرية للعناصر الثقيلة، وتحديدًا الذهب (Au) والأستاتين (At) والتينيسين (Ts) مع أيوناتها (±1) باستخدام هاملتونيات ZORA وSchrödinger وعلى مستوى Hartree-Fock (HF). تغطي الدراسة حساب أنصاف الأقطار وطاقات التأين والإستقطابيات. توضح الدراسة أثر إمتداد القاعدة dyall.npz (n= D, T, Q) المستعملة في الحساب. تشير النتائج إلى اتفاق جيد للإستقطابيات مع القيم التجريبية في الحالة النسبوية باستخدام dyall.4zp. تظهر أنصاف الأقطار أيضًا توافقا ممتازًا مع القيم النظرية النسبوية الأخرى باستخدام القاعدة dyall.nzp. يُلاحظ بشكل لافت توسع السبينور $p_{3/2}$ في ذرات الأستاتين والتينيسين بفعل التأثيرات النسبوية، مما يشير إلى تأثيرات محتملة على أطوال الروابط في الجزيئات ذات الصلة. علاوة على ذلك، تقدم هذه الدراسة حسابات للمرة الأولى تتعلق بخصائص أيونات الأستاتين والتينيسين، مما يثري فهمنا لهذه العناصر الثقيلة.

الكلمات المفتاحية: الذهب، الأستاتين، التينيسين، نصف القطر الذري، طاقة التأين، الأستقطابية، هاملتوني ZORA.

I- Introduction:

Contemporary theoretical physics is built upon two cornerstone theories: quantum mechanics and special relativity. Special relativity posits that the mass (m) of a particle grows relative to its rest mass (m_0) with increasing speed. This phenomenon becomes significant only when the particle's speed approaches the speed of light (c). Notably, this is observed in electrons situated near the nucleus of heavy elements. The influence of relativistic effects causes a reduction in the radii of electron orbitals close to the nucleus. A qualitative understanding of this phenomenon can be derived from a straightforward argument, which is as follows:

$$\mathbf{m = m_0 / (1 - (\vartheta/c))^{1/2} \ldots\ldots (1)}$$

The effective Bohr radius, denoted as $a_0 = (4\pi\varepsilon_0)(\hbar^2/m_e^2)$, experiences a reduction for inner electrons exhibiting higher average speeds. Traditionally, the outermost electrons dictate the chemical behavior of an element. This led Dirac to assert in 1929 that "Relativistic effects are therefore of no importance in the consideration of atomic and molecular structure and ordinary chemical reactions" [1]. However, it has been subsequently revealed that relativistic effects, initially deemed inconsequential for outer orbitals, can have more significant implications [2,3]. The contraction of inner electron shells in multi-electron atoms can indeed impact the characteristics of valence orbitals. The external orbitals may undergo either expansion or contraction, contingent upon alterations in the screening of the underlying inner orbitals, as the relativistic effects within the inner shell influence the atomic field's self-consistency requirement [4]. Our research focuses on a theoretical examination of ionization potentials, polarizabilities, and atomic radii for Gold ($_{79}$Au), Astatine ($_{85}$At), and Tennessine ($_{117}$Ts) atoms, along with their ions carrying charges of 1, 0, and -1. Although previous studies have explored these properties, particularly for gold, and to a lesser extent for Astatine and Tennessine, our work contributes by utilizing various theoretical levels and calculation parameters, including different Hamiltonians (ZORA, DKH, DC, etc.), electron treatment methods (all electron, effective core potential), spinor components (1C, 2C, or 4C), calculation methods (HF, MP2, CI, CC for wave function-based method; LDA, B3LYP for density functional-based method), nuclear model charge distributions (Nucleus point, Finite nucleus (Uniform Sphere, Fermi, Gaussian)), and diverse basis sets. We employ a distinct theoretical approach in our study. Gold is known to be a heavy element, and relativistic effects are recognized as essential in its behavior. Astatine and Tennessine are both part of the halogen group, renowned for their heightened electro-negativity. Furthermore, Gold and Astatine share the same row in the periodic table. This prompts an exploration into how relativistic effects evolve within the same row when transitioning from one heavy atom (Au) to another (At). Additionally, by keeping Gold constant and transitioning from Astatine to eka-Astatine (Ts) within the same column, we aim to comprehend the variations in relativistic effects.

II- Computational details

All computations in this study were executed using the DIRAC code, version 2023 [5]. We adopted the scaled ZORA (Zeroth Order Regular Approximation) Hamiltonian [6,7,8] normalized over 4-components to account for relativistic effects, while the Schrödinger Hamiltonian was employed for non-relativistic calculations. For all-electron calculations, the Hartree-Fock (HF) level was utilized, employing the dyall.nzp basis set (where n = D, T, Q) [9], and incorporating a nuclear Gaussian charge distribution model [10].

III- Results and discussion

In this segment, we present the computed atomic properties for X^n systems, where X represents Au, At, and Ts, and n denotes 0, -1, or +1. The atomic properties under scrutiny include radii (R), ionization energies (IE), and polarizabilities (α). To assess the dimensions of the valence orbitals, we determined the rms $<r^2>^{1/2}$ by summing $<x^2>$, $<y^2>$, and $<z^2>$. Ionization energies were derived using the formula $IE = E(A^+) - E(A^0)$. In both relativistic and non-relativistic calculations, the numerical finite field technique (FFT) [11] was employed for calculating polarizabilities in open shell systems. Electric field strengths of 0.000, ±0.0005, and ±0.001 were utilized. For closed-shell systems in the non-relativistic case, FFT was applied, while for closed-shell systems in the relativistic case, the analytical response theory was implemented [12]. Table 1 presents the aforementioned atomic properties obtained at the HF level using the dyall.2zp basis set, considering both relativistic and non-relativistic cases.

Table 1: Radii (Å), Ionization Energies (eV), and Polarizabilities (a.u.) for Au, At, and Ts atoms and their ions, as determined by the HF method employing the dyall.2zp basis set.

S	H	R	IP	α	S	R	α	S	R	α
Au	NR	2.014	5.878	94.15	Au^-	2.128	156.9	Au^+	0.878	9.990
	NR[15]	1.96								
	R	1.741	7.643	46.21		1.907	96.56		0.911	11.51
	R[15]	1.62								
	EXP		9.217[a]	49.1 ± 4.1[b] 39.1 ± 9.8						
At	NR	1.523	9.816	19.80	At^-	1.584	21.52	At^+	1.457	17.80
	R	1.537	9.867	19.43		1.605	22.23		1.463	16.42
	R[16]	1.56				1.63			1.44	
	EXP		9.21	42 ± 4[b]						
Ts	NR	1.693	9.131	26.01	Ts^-	1.754	27.98	Ts^+	1.626	27.84
	R	1.744	10.11	25.03		1.821	28.57		1.658	21.03
	R[16]	1.80				1.99			1.63	
	rec			76 ± 15[b]						

[a] Ref [13], [b] Ref [14], The value of polarizability of Ts atom is the recommended value.

In interpreting Table 1, our analysis aligns with the findings of [17], which state that "The relativistic effect is apparent in the radial contraction of penetrating s and p shells, and expansion of non-penetrating d and f shells.". Our results for all systems involving gold corroborate with [17], indicating that the radii of neutral and anionic gold experience a reduction of approximately 14% and 10%, respectively, during the transition from non-relativistic to relativistic cases. This contraction is attributed to the s-type orbital characteristics of these systems. Conversely, in the case of the gold cation, our findings reveal an increase of approximately 4% in atomic radii when passing from non-relativistic to relativistic cases. This stands in contrast to the radial contraction observed for gold's neutral and anionic forms, and it is notable that this deviation aligns with the distinctive behavior of cations. However, our results for the At and Ts systems diverge from the expectations outlined in [17]. Despite both systems terminating with the $6p_{3/2}$ and $7p_{3/2}$ spinors, respectively, we observe an expansion in atomic radius. This discrepancy suggests that factors beyond the specific spinors play a role in determining the relativistic effects on these systems. Furthermore, in the case of the gold atom, our calculated contraction of 14% contrasts with the 17% contraction predicted by reference [14]. This variance emphasizes the sensitivity of relativistic effects to specific computational methodologies and parameters. The work by Chang et al. [15] lacks non-relativistic calculations for the atomic radius of Astatine (At) and Tennessine (Ts), making it challenging to gauge the significance of relativistic effects in their findings. In our study, we can quantify these effects. For neutral, anionic, and cationic astatine, we observe minimal atomic radius expansions of only 0.9%, 1.3%, and 0.4%, respectively. However, these values increase to 3%, 3.8%, and 2.0%, respectively, for the Tennessine system. Notably, the importance of relativistic effects follows the order cationic → neutral → anionic for both At and Ts. Furthermore, this trend aligns with the percentage of occupancy in the outermost electronic sub-shell p, which increases for both At and Ts atoms in the sequence: 66% → 83% → 100%. Additionally, we observe a greater percentage of expansion for Ts compared to At, attributable to the higher nuclear charge of Ts.

The impact of relativistic effects on the outermost orbital radius in gold is more pronounced compared to their effect on the outermost spinors in astatine and tennessine, despite the latter two being heavier elements. Drawing from these observations, one can infer how relativistic effects influence the ionization energies of the studied atoms. In theory, the relativistic ionization energy should be higher than the non-relativistic ionization energy for gold and lower for astatine and tennessine. However, our calculations reveal that relativistic effects lead to an increase in the ionization potentials of At and Ts atoms. This unexpected outcome can be attributed to the fact that the calculated radii correspond to the $p_{3/2}$ spinors, while the energies were computed for the average energy of six states: $(2.\ E_{p1/2} + 4.\ E_{p3/2})/6$: This discrepancy becomes evident in Figure 1, which illustrates a significant contraction in the $p_{1/2}$ spinor due to relativistic effects, contrasting with a relatively smaller expansion in the $p_{3/2}$ spinors. Consequently, the instability induced by relativistic effects in the $p_{3/2}$ spinors is counteracted by increased stability in the $p_{1/2}$ spinor, resulting in an overall higher ionization potential.

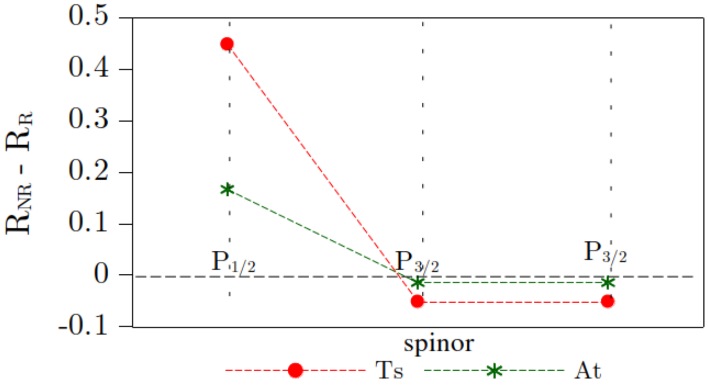

Figure 1.

In comparing the ionization potential values for the examined atoms, we observe a sequential increase influenced by relativistic effects, with the order being At → Ts → Au. This order aligns with the observed trend in radii as well. Supplementary theoretical ionization potential values are detailed in Table 2.

Table 2: Alternative Theoretical Values for Ionization Energy (eV).

system	NR	R
Au	6.98^{a1}, 5.92^{b1},	9.10^{a2}, 9.09^{a3}, 7.65^{b2},
At		9.04^{c}
Ts		7.31^{c}

[a] Ref [18], [b] Ref [19], [c] Ref [16]. a_1, a_2 and a_3 are the results of correlated coupled-cluster using non-relativistic, Dirac-Fock-Coulomb and Dirac-Fock-Breit Hamiltonians, Respectively. b_1, b_2, non-rel. Self-consistent field and rel. I-camp. self-consistent field, respectively. c the values according to the multi-configuration Dirac-Fock (MCDF) method.

As indicated in Table 2, non-relativistic values for At and Ts atoms are absent, limiting the ability to discuss the significance of relativistic effects. This study provides predictions for these effects. Comparisons are drawn between values obtained through the non-correlated HF theory and those from reference [18], which utilized the more accurate correlated coupled cluster theory. This comparison aids in understanding the joint impact of correlation and relativistic effects. An essential objective of this study is to underscore the significance of relativistic effects independently of correlation effects. Conversely, when contrasting our results, both relativistic and non-relativistic, with those from reference [19], a satisfactory agreement is observed. This agreement is attributed to the similar levels of theory employed in both studies. Notably, there is a substantial level of agreement for the astatine atom, although less so for the tennessine atom.

Table 1 illustrates a 7% deviation from the experimental ionization potential for the Astatine (At) atom, indicating reasonably good agreement with experimental values. Table 2 reveals a decrease in this deviation to 2%, which aligns with expectations, considering the higher precision of the MCDF method used in comparison to the method employed in this study. Additionally, it's noteworthy that the value from reference [16] pertains to a specific state of the atom, while our value is an average across different configuration states. For the Tennessine (Ts) atom, lacking an experimental ionization potential value, we utilize the more precise theoretical value from reference [16] as a reference point for calculating the percentage deviation due to relativistic effects. This calculation results in a 38% discrepancy with the value from reference [16].

When a homogeneous static electric field, denoted as $F = [F_x, F_y, F_z]$ with p, q-components, is applied to a physical system, its energy can be expressed through a Taylor series expansion, employing Einstein's summation convention, as follows:

$$E = E_0 - \mu_p F_p - (\tfrac{1}{2})\,\alpha_{pq} F_p F_q \text{ .....(2)}$$

The polarizability, specifically the zz-component, is determined by taking the second numerical derivative of the energy concerning the electric field, specifically at zero field strength:

$$\alpha_{zz} = -(\partial^2 E\,(F_z)/\partial F_z^2)_{F_z = 0} \text{ .....(3)}$$

For atoms, the diagonal components of the polarizability tensor are identical due to symmetry. The polarizability values for the analyzed systems, computed using various basis sets, are presented in Tables 1, 3, and 4.

Table 3: Radii (Å), Ionization Energies (eV), and Polarizabilities (a.u.) for Au, At, and Ts atoms and their ions, as determined by the HF method employing the dyall.3zp basis set.

S	H	R	IP	α	S	R	α	S	R	α
Au	NR	2.086	5.914		Au^-	2.415		Au^+	0.877	
	R	1.744	7.686	47.48		2.061	158.2		0.912	12.33
	EXP		9.217[a]	49.1 ± 4.1 39.1 ± 9.8						
At	NR	1.528	9.739		At^-	1.642		At^+	1.438	
	R	1.548	10.85	30.68		1.702	41.83		1.447	22.08
	EXP		9.21	42 ± 4						
Ts	NR	1.680	9.057		Ts^-	1.799		Ts^+	1.587	
	R	1.780	10.09	45.65		1.983	61.68		1.629	31.85
	rec			76 ± 15						

In contrast to the atomic radius and ionization potential, where the choice of basis set has a relatively minor impact, the polarizability is highly sensitive to this choice. To better understand the variations in polarizabilities for the studied atoms concerning both experimental values and those obtained with different basis sets, Figure 2 is provided. Analyzing the effect of the basis set, it becomes evident that, for the gold atom, all theoretical values fall within the range of experimental ones, even with the less extensive dyall.2zp basis set. Additionally, it is apparent that the influence of the basis set on the polarizability of gold remains modest. However, for both Astatine (At) and Tennessine (Ts) atoms, the impact of the basis set is more pronounced compared to the gold atom. This suggests that the super-heavy character is more susceptible to the choice of basis set than its heavier counterpart.

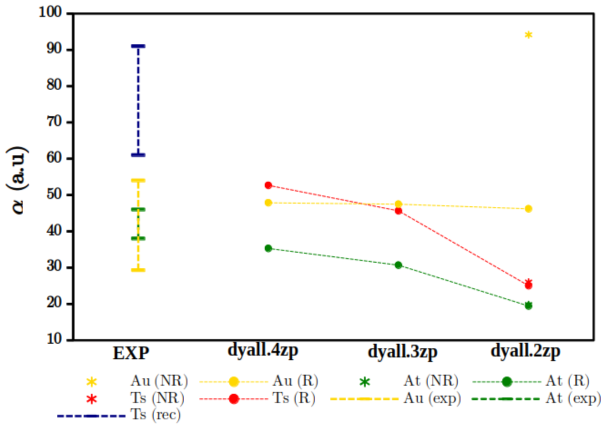

Figure 2.

For the Astatine (At) atom, the theoretical polarizability value obtained with the dyall.4zp basis set is nearly within the range of experimental values. In contrast, the theoretical values obtained with the dyall.2zp and dyall.3zp basis sets fall outside the interval of experimental values. Similar behavior is observed for the Tennessine (Ts) atom in terms of disagreement with the recommended polarizability value. This disagreement becomes more pronounced with a less extended basis set. Moreover, it is established that polarizability is inversely proportional to the ionization potential [20]. Comparing the non-relativistic and relativistic polarizabilities, as well as the non-relativistic and relativistic ionization potentials for the three atoms calculated using the dyall.2zp basis set, we observe adherence to this rule. Interestingly, this rule is violated when transitioning to more extended basis sets like dyall.3zp and dyall.4zp. Figure 2 reveals a crucial finding: relativistic effects exert a significant impact on the polarizability of gold, while their influence on Astatine and Tennessine atoms is notably weaker, despite the latter two being heavier elements. This observation aligns well with the trends observed for atomic radii and ionization potential.

Table 4: Radii (Å), Ionization Energies (eV), and Polarizabilities (a.u.) for Au, At, and Ts atoms and their ions, as determined by the HF method employing the dyall.4zp basis set.

S	H	R	IP	α	S	R	α	S	R	α
Au	NR	2.106	5.915		Au^-	2.627		Au^+	0.877	
	R	1.744	7.688	47.87		2.147	158.2		0.912	12.35
	EXP	0.000	9.226	49.1 ± 4.1 39.1 ± 9.8						
At	NR	1.528			At^-	1.658		At^+	1.437	
	R	1.557	9.840	35.29		1.739	53.90		1.446	23.63
	EXP		9.21	42 ± 4						
Ts	NR	1.679			Ts^-	1.814		Ts^+	1.586	
	R	1.781	10.08	52.67		2.069	77.63		1.627	34.10
	Rec			76 ± 15						

By examining Figure 3 and referring to Table 4, we elucidate the impact of adding or removing an electron from an atom X on its polarizability, where X represents Au, At, and Ts atoms. Notably, we observe a decrease in polarizability following the order $X^- \rightarrow X \rightarrow X^+$. This behavior aligns with Schwerdtfeger's observation, as indicated by a comparison of ionization energies for the three systems X^-, X, and X^+.

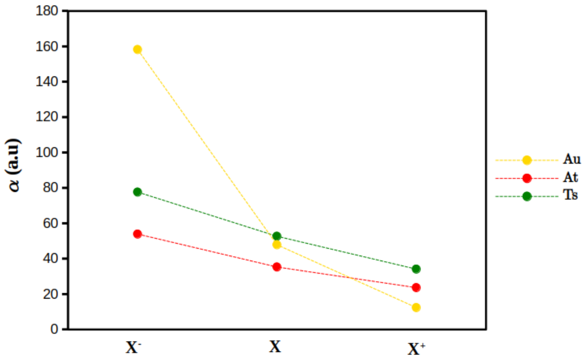

Figure 3

Table 5 compiles several theoretical values for the polarizabilities of the gold atom and its ions. As far as our knowledge extends, there are no available experimental or theoretical values for the polarizabilities of astatine and tennessine anions. Regarding the astatine neutral systems, several values have been reported (in atomic units): 45.6 for the state $^{2}P_{1/2}$, and 43.0, 40.7 ± 2.0, 38.93, 38.15, 40.4, 41.1 for the state $^{2}p_{3/2}$. For the tennessine atom, empirical estimates include 76.3 and 54.24 (estimated via correlation with Rmax ($np_{3/2}$)) for the state $^{2}p_{3/2}$ [14], with the latter value closely resembling our calculated result.

Table 5: Other theoretical vales of polarizability (a.u.) for gold atom and it's ions.

	+1	0	-1
HF	**10.59**	**46.70**	**205.0**
	9.043	103.7	660.1
MP4	**11.67**	**31.18**	**60.60**
	9.785	50.48	279.6
QCISD(T)	**11.61**	**35.09**	**96.03**
	9.650	64.11	257.1

All values were taken from the reference [21], relativistic values are given in bold. HF: unrestricted Hartree-Fock, MP2 : Moller-Plesset second-order procedure, QCISD(T): quadratic configuration interaction estimating triple contributions.

Conclusion

Our study on the atomic properties of heavy elements, including Gold (Au), Astatine (At), and Tennessine (Ts), along with their ions, yielded valuable insights. The examination of radii, ionization energies, and polarizabilities using both ZORA and Schrödinger Hamiltonians at the HF level, along with the exploration of basis set size impact, provided significant findings. Notably, good agreement with experimental values for polarizabilities was observed in the relativistic case with the dyall.4zp basis set, while the excellent agreement with other theoretical values for radii was noted in the relativistic scenario with dyall.nzp basis sets. Gold displays more marked relativistic effects than astatine and tennessine, despite being lighter. The study also highlighted the expansion of $p_{3/2}$ spinors in Astatine and Tennessine atoms due to relativistic effects, suggesting potential implications for bond lengths in molecules containing these elements. Additionally, this research contributed novel calculations related to astatine and tennessine ions, filling a gap in the existing literature. Overall, the study enhances our understanding of the intricate atomic properties of heavy elements and their ions.

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