

# Atomic Structure of $\text{Nd}^{9+}$ for Highly Charged Ion Clocks

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**Abstract:** The energy levels arising from the electronic orbital  $5p - 4f$  crossing between the ground  $5p^2 4f$  and excited  $5p 4f^2$  configurations in the  $\text{Nd}^{9+}$  ion are investigated by using high-accuracy relativistic ab initio calculations. The accurate atomic data of the lifetime,  $g_J$  factor, electric quadrupole moment, and hyperfine structure of the magnetic dipole are also presented. The long-lived states that are suitable for making narrow-linewidth (milli-Hz) clock lines are found. Dominant systematics caused by stray electromagnetic interactions in an experiment and the coefficients of the relativistic sensitivity to variation of the fine-structure constant  $\alpha$  and of the Lorentz invariance violation are evaluated, thus validating that the  $\text{Nd}^{9+}$  ion can be a new candidate for high-resolution spectroscopy and precision fundamental studies for probing new physics beyond the Standard Model.

**Keywords:** energy level;  $5p-4f$  crossing;  $\text{Nd}^{9+}$  ion; highly charged ion clocks; multi-reference configuration interaction; CI+MBPT; lifetimes; magnetic-dipole hyperfine structure constant; electric dipole polarizability; variation of  $\alpha$ ; violation of the local Lorentz invariance



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## 1. Introduction

Highly charged ion (HCI) clocks have been suggested to be some of the most interesting candidates for future frequency metrology, with the aim of breaking precision limits lower than  $10^{-18}$  and aiding in the quest for powerful tools to be used research in physics beyond the Standard Model. The experimental advances in fabrication, cooling, and trapping of highly charged ions have enabled the measurement of the optical spectroscopy of several categories of highly charged ions, such as Nd-like ions [1], the  $\text{Ho}^{14+}$  ion [2], the  $\text{Pr}^{9+}$  ion [3], the  $\text{Ni}^{11+}$ - $\text{Ni}^{14+}$  ions [4], etc. Very recently, the sympathetic cooling and the coherent laser spectroscopy of  $\text{Ar}^{13+}$  were demonstrated [5]. All of this progress makes HCIs accessible for high-resolution spectroscopy and precision fundamental studies.

HCIs have high sensitivities to variations in fundamental constants as a consequence of their strong relativistic effects and higher ionization energies. Such high sensitivities can be further enhanced by the electronic-orbital-crossing phenomenon that occurs in inter-configurations. As an Sb-like lanthanide ion, the  $\text{Nd}^{9+}$  ion has the core  $[1s^2, \dots, 4d^{10}, 5s^2]$  and three valence electrons in the  $5p$  and  $4f$  shells. The reordering of the  $5p$  and  $4f$  electronic orbital binding energies along the Sb-like isoelectronic sequences generates rich optical transitions over inter-configurations. However, the energy levels due to such

$5p - 4f$  crossings may be very complicated. In particular, the  $5s$  orbital has a binding energy that is close to those of the  $5p$  and  $4f$  shells. This indicates that the two  $5s$  electrons should be included in the valent field, considering the  $\text{Nd}^{9+}$  ion as a five-valent system. For many-electron valent systems, the configuration interaction method (CI) is a widely adopted method, and, in principle, it has no limit for the number of valence electrons. However, calculations of many-valence-electron systems have many practical difficulties in terms of their computational techniques, especially when the number of valence electrons is beyond 4. The accurate prediction of the optical transition in HCIs with valence electrons in the  $4f$  shell is especially challenging. Berengut et al. studied the  $4f-5p$  level crossing in  $\text{Nd}^{9+}$  [6]. Complete and consistent information about  $\text{Nd}^{9+}$  ions remains scarce.

In this work, we adopted two different CI methods—the multi-reference configuration interaction (MRCI) method [7–9] and the configuration interaction plus many-body perturbation theory (CI+MBPT) theory [10,11]. The comparative computation based on the MRCI and CI+MBPT methods ensures the consistency and reliability of our predicted results with minimal uncertainty. Our results show that the  $5p-4f$  crossing generates wealthy laser-accessible states over the  $5p^24f$  and  $5p4f^2$  configurations. The long-lived states that are suitable for making clocks are identified. Accurate data on the atomic properties, such as energies, lifetimes, the  $g_J$  factor, the magnetic-dipole hyperfine structure (hfs) constants, and the electric quadrupole moment, are predicted. The clock-transition-related properties are calculated, thus validating the dominant systematics that are attainable to below  $10^{-19}$ . High coefficients of the relativistic sensitivity to variations in the fine-structure constant  $\alpha$  and the violation of the local Lorentz invariance are found for the clock transitions of  $\text{Nd}^{9+}$ , indicating its application to studies of a possible varying fine-structure constant  $\alpha$  and the violation of the local Lorentz invariance.

## 2. Computational Methods

### 2.1. MRCI

The calculations start with the Dirac–Hartree–Fock (DHF) calculation under the Dirac–Coulomb–Gaunt Hamiltonian that is given by

$$\hat{H} = \sum_i [c(\vec{\mathbf{f}} \cdot \vec{\mathbf{p}})_i + (\beta - 1)_i m_0 c^2 + V_{iA}] + \sum_{i < j} \left[ \frac{1}{r_{ij}} - \frac{1}{2} \frac{\vec{\mathbf{f}}_i \cdot \vec{\mathbf{f}}_j}{r_{ij}} \right], \quad (1)$$

where  $\vec{\mathbf{f}}$  and  $\beta$  are Dirac matrices,  $\vec{\mathbf{p}}$  is the kinetic momentum,  $m_0 c^2$  is the resting mass energy of an electron with the speed of light  $c$ ,  $V_{iA}$  is the nuclear potential with the atomic mass number  $A$ , and  $r_{ij}$  is the distance between the  $i$ -th and  $j$ -th electrons. The last term in Equation (1) is the Gaunt term, which is the leading term of the Breit interaction. The DHF calculation is combined with the relativistic all-electron correlation-consistent optimized basis sets developed by Dyall et al., which contain the {24s;19p;13d;8f;2g}, {30s;24p;16d;11f;3g;2h}, and {35s;30p;19d;13f;5g;3h;2i} functions in the  $2\zeta$ ,  $3\zeta$ , and  $4\zeta$  basis sets, respectively [12].

Based on the single-electron wavefunctions obtained with the DHF calculation, a string-based Hamiltonian-direct configuration interaction [7–9] calculation was carried out. The electron excitation from the occupied to the virtual orbitals comprised configuration spaces with different sizes by tailoring the numbers of the active electrons and the correlated orbitals to balance the computational cost and accuracy. The maximum of 28 electrons that occupied the  $3d$ ,  $4s$ ,  $4p$ , and  $4d$  orbitals were set in order to allow for a single (S) excitation; five electrons in the  $5s$ ,  $5p$ , and  $4f$  shells were assigned to be valence electrons for single and double (SD) excitations; virtual orbitals with energy less than 10 a.u. were included in the CI space, which contained  $9sp8df6g$  (which indicates  $s$ - and  $p$ -orbitals with  $n \leq 9$ ,  $d$ - and  $f$ -orbitals with  $n \leq 8$ , and  $g$ -orbitals with  $n \leq 6$ ) in the  $2\zeta$  basis set,  $10sp9df6g7h$  in the

$3\zeta$  basis set, and  $12sp10df7ghi$  in the  $4\zeta$  basis sets. The MRCI calculations were performed by using a relativistic ab initio electronic structure program, DIRAC [13].

## 2.2. CI+MBPT

The CI+MBPT calculation is based on the Dirac–Coulomb–Breit Hamiltonian, which is similar to Equation (1), with the one-electron Dirac–Fock operator

$$h_{DF} = c(\vec{\mathbf{f}} \cdot \vec{\mathbf{p}})_i + (\beta - 1)_i m_0 c^2 - \frac{Z}{r} + V^{N_{DF}}(r), \quad (2)$$

and the Breit term

$$B_{ij} = -\frac{1}{2r_{ij}}(\vec{\mathbf{f}}_i \cdot \vec{\mathbf{f}}_j + (\vec{\mathbf{f}}_i \cdot \vec{\mathbf{r}}_{ij})(\vec{\mathbf{f}}_j \cdot \vec{\mathbf{r}}_{ij})/r_{ij}^2), \quad (3)$$

where  $V^{DF}$  is the potential of the  $N_{DF}$  electrons included in the self-consistent DHF procedure. Herein,  $N_{DF}$  is either all  $N$  electrons of the atom or some subset of them. The choice of the potential may impact the calculation results. The QED interaction is included by adopting the radiative potential method, which was originally developed by Flambaum and Ginges [14]. The remaining valence and virtual orbitals (pseudostates) are constructed as a linear combination of B-spline basis functions. The configuration space is constructed by allowing SD excitation from the leading configurations,  $5s^25p^24f$  and  $5s^25p4f^2$ , up to  $8spdf$ , alongside the entirety of the SD excitations from the  $4d$  shells for the large-side CSFs, while the small-side CSFs are restricted to  $6spdf$  for the SD excitations and  $8spdf$  for an additional S excitation. Correlations with the frozen core orbitals, i.e., those below  $4d$  and the virtual orbitals beyond the valence basis set, are treated using the second-order MBPT. The B-spline basis set includes virtual orbitals up to the main quantum number  $n \leq 30$  and angular momentum  $l \leq 4$ . We use the ‘use-valence’ flag to include valence–valence MBPT diagrams for orbitals above the valence basis set and below the MBPT basis set. The CI+MBPT calculation was carried out by using the AMBiT code [11].

## 3. Energy Levels

The excited energies (EEs) of the low-lying states in  $\text{Nd}^{9+}$  obtained with the MRCI calculation are shown in Table 1. We first adopt an intermediate CI model space that correlates 18 core electrons ( $4s^24p^64d^{10}$ ) at the S-excitation level and five valence electrons of the  $5s, 5p, 4f$  shells at the SD-excitation level; these are referred to as ‘(core18) $_{2\zeta}$ ’, ‘(core18) $_{3\zeta}$ ’, and ‘(core18) $_{4\zeta}$ ’ for the different basis sets. The convergent energy values are obtained at the  $4\zeta$  basis set with a possible error due to the finite-size effect of the basis set, with  $\Delta_{basis}$  being estimated by the difference between (core18) $_{3\zeta}$  and (core18) $_{4\zeta}$ . Two additional calculations are conducted for the  $2\zeta$  basis set: The first calculation includes the triple excitations of the  $5s, 5p, 4f$  valence electrons, referred to as ‘(core18) $^T$ ’; this is used to estimate the possible correction due to the triple excitations,  $\Delta_T$ , through the difference between ‘(core18)’ and ‘(core18) $^T$ ’; the second calculation extends the inner-core excitations up to the inclusion of 28 core electrons by adding those from the  $3d$  shell, referred to as ‘(core28)’; then, the correction due to more core excitations,  $\Delta_c$ , is estimated by the difference between ‘(core18)’ and ‘(core28)’. The contribution of the QED interaction,  $\Delta_{QED}$ , that is absent in the MRCI calculation is taken from the AMBiT calculation. The final results are recommended based on (core18) $_{4\zeta}$  plus  $\Delta_{QED}$ , with the corresponding uncertainties assigned according to the rms of  $\Delta_{basis}$ ,  $\Delta_T$ , and  $\Delta_c$ .

**Table 1.** The excited energies (EEs) ( $\text{cm}^{-1}$ ) of the energy levels in the  $\text{Nd}^{9+}$  ion obtained with the MRCI calculation.

Levels	(core18) <sub>2ξ</sub>	(core28) <sub>2ξ</sub>	(core18) <sub>2ξ</sub> <sup>T</sup>	(core18) <sub>3ξ</sub>	(core18) <sub>4ξ</sub>	$\Delta_{QED}$	$\Delta_{basis}$	$\Delta_T$	$\Delta_c$	Final	Unc.
G0: $(5p^24f)_{5/2}^0$	0	0	0	0	0	0	0	0	0	0	0
G1: $(5p^24f)_{7/2}^0$	6568	6528	6513	6569	6583	20	15	−55	−40	6524	69
E0: $(5p4f^2)_{9/2}^0$	17,352	16,606	16,649	19,142	20,662	−140	1521	−703	−746	20,594	1834
E1: $(5p4f^2)_{7/2}^0$	20,484	19,953	19,780	22,114	23,243	−81	1129	−704	−531	23,056	1432
E2: $(5p4f^2)_{11/2}^0$	23,687	23,081	22,903	25,859	27,306	−112	1446	−784	−606	27,249	1753
E3: $(5p4f^2)_{9/2}^0$	23,977	23,392	23,206	26,156	27,553	−95	1397	−770	−585	27,501	1699
E4: $(5p4f^2)_{5/2}^0$	25,615	25,032	25,463	27,728	29,039	−59	1311	−152	−582	29,557	1443
E5: $(5p4f^2)_{3/2}^0$	26,494	26,052	26,361	28,727	29,916	−52	1190	−132	−442	30,479	1276
E6: $(5p4f^2)_{7/2}^0$	27,744	27,139	27,243	29,645	30,968	−44	1323	−501	−605	31,140	1539
E7: $(5p4f^2)_{11/2}^0$	28,061	27,446	27,403	30,327	31,748	−69	1420	−658	−615	31,826	1682
E8: $(5p4f^2)_{5/2}^0$	29,158	28,633	28,964	31,155	32,377	−90	1222	−194	−525	32,790	1344
E9: $(5p4f^2)_{13/2}^0$	29,839	29,372	29,015	32,352	33,713	−101	1361	−824	−467	33,681	1658

The EEs obtained by the CI+MBPT calculations are given in Table 2. The changes in the EEs under the  $V^{N-5}$ ,  $V^{N-3}$ , and  $V^N$  potentials are obvious, more than 2000–3000  $\text{cm}^{-1}$ , bringing in certain uncertainty. The  $\Delta_n$  considers the changes in the EEs when the valence basis set increases to  $10spdf$ . The final results are given using the results under the  $V^N$  potential plus  $\Delta_{QED}$  and  $\Delta_n$ .

**Table 2.** The excited energies (EEs) ( $\text{cm}^{-1}$ ) of the energy level in the  $\text{Nd}^{9+}$  ion obtained with the CI+MBPT calculations.

Level	$V^{N-5}$	$V^{N-3}$	$V^N$	$\Delta_{QED}$	$\Delta_n$	Final
G0: $(5p^24f)_{5/2}^0$	0	0	0	0	0	0
G1: $(5p^24f)_{7/2}^0$	6026	6115	6064	20	−2	6062
E0: $(5p4f^2)_{9/2}^0$	23,049	21,729	19,702	−140	349	20,072
E1: $(5p4f^2)_{7/2}^0$	24,519	23,266	22,472	−81	178	22,510
G2: $(5p^24f)_{5/2}^0$	26,895	26,359	26,607	−95	−36	26,490
E2: $(5p4f^2)_{11/2}^0$	28,831	27,597	25,471	−112	350	25,710
E3: $(5p4f^2)_{9/2}^0$	29,131	27,622	25,880	−95	324	26,110
E4: $(5p4f^2)_{5/2}^0$	31,316	30,180	28,439	−59	190	28,570
E5: $(5p4f^2)_{3/2}^0$	28,892	28,110	27,464	−52	290	27,702
E6: $(5p4f^2)_{7/2}^0$	30,553	29,770	287,38	−44	243	28,937
E7: $(5p4f^2)_{11/2}^0$	33,434	32,054	29,917	−69	324	30,172
E8: $(5p4f^2)_{5/2}^0$	33,159	31,793	30,539	−90	132	30,582
E9: $(5p4f^2)_{13/2}^0$	35,055	33,999	32,785	−101	187	32,871

The MRCI and CI+MBPT results for the EEs are consistent within a reasonable error range. The EE results prove that the  $\text{Nd}^{9+}$  ion has a  $5p^24f$  ground configuration. The fine-structure splitting via  $(5p^24f)_{5/2}^0$  and  $(5p^24f)_{7/2}^0$ , labeled as G0 and G1, respectively, is around 6524(69)  $\text{cm}^{-1}$  (MRCI result), which is consistent with the earlier calculations [6,15]. Subsequently, the  $5p - 4f$  orbital crossing raises many of the  $5p4f^2$  excited states for those below about 30,000  $\text{cm}^{-1}$ , which are listed as E0 to E9 in Tables 1 and 2. Another fine-structure splitting state for the ground configuration, G2:  $5p^24f$ , is found in the CI+MBPT calculation.

#### 4. The Atomic Properties

Table 3 compares the results obtained with MRCI and AMBiT for the lifetime  $\tau$ ,  $g_j$  factor, electric quadrupole moment  $\Theta$ , and magnetic-dipole hyperfine structure constant  $A$  for the energy levels in the  $\text{Nd}^{9+}$  ion. The differences in level energies of the MRCI and AMBiT results change the transition wavelengths and then lead to differences in the  $\tau$  values. The results for  $\tau$  justify several long-lived excited states that are suitable for making clock transitions. One good example is the G0:  $(5p^24f)_{5/2}^0 - E0: (5p4f^2)_{9/2}^0$  transition,

which occurs at 485 (80) nm (the MRCI result) and has a natural linewidth that is estimated to be about 2 milli-Hz in terms of the 67.21 s (the MRCI result) upper-state lifetime. In the case of the odd isotope, hyperfine mixing with faster decaying levels may need to be taken into account, as it can change the lifetime of  $E0 : (5p4f^2)_{9/2}^o$ , or we can choose appropriate hyperfine sublevels  $F$  to adjust the hyperfine–mediate transitions. The results for the  $g_j$  factor and the electric quadrupole moment  $\Theta$  (a.u.), as they show excellent consistency between the MRCI and CI+MBPT calculations, are used for the evaluation of the systematic effect of the clock transition. The Nd element has rich, naturally stable isotopes— $^{142,143,144,145,146,148,150}\text{Nd}$ . The even isotopes have simple energy levels, which is advantageous for setting up the clock transition, whereas the hyperfine structures also have a wide range of usage for atomic clocks. For completeness, we provide the hyperfine structure constant  $A$  (MHz) of  $^{143}\text{Nd}^{9+}$  (nuclear spin  $I = 3/2$  and nuclear magnetic moment  $\mu_I = -1.08\mu_N$ , where  $\mu_N$  is a nuclear magneton), which has the greatest natural abundance. Table 4 lists some clock-transition-related properties.

**Table 3.** Comparison of the lifetime  $\tau$  (s),  $g_j$  factor, electric quadrupole moment  $\Theta$  (a.u.), and magnetic-dipole hyperfine structure constant  $A$  (MHz) of the energy levels in the  $\text{Nd}^{9+}$  ion obtained with the MRCI and AMBiT calculations.

Level	$\tau$ (s)		$g_j$		$\Theta$ (a.u.)		$A$ (MHz)	
	MRCI	AMBiT	MRCI	AMBiT	MRCI	AMBiT	MRCI	AMBiT
G0: $(5p^24f)_{5/2}^o$			0.830	0.837	0.019	0.006	−376	−352
G1: $(5p^24f)_{7/2}^o$	0.17	0.47	1.157	1.155	−0.044	−0.009	−175	−169
E0: $(5p4f^2)_{9/2}^o$	67.21	49.55	0.808	0.815	−0.103	−0.101	−1086	−1042
E1: $(5p4f^2)_{7/2}^o$	0.05	0.04	0.829	0.863	0.082	0.082	2	86
E2: $(5p4f^2)_{11/2}^o$	0.11	0.46	1.011	1.014	0.076	0.064	−854	−814
E3: $(5p4f^2)_{9/2}^o$	0.40	0.16	1.040	1.048	−0.098	−0.091	192	228
E4: $(5p4f^2)_{5/2}^o$	0.04	0.004	0.676	0.689	0.032	0.023	−1352	−1326
E5: $(5p4f^2)_{3/2}^o$	0.15	0.05	0.726	0.897	−0.034	−0.032	1215	1051
E6: $(5p4f^2)_{7/2}^o$	0.02	0.01	1.018	1.007	−0.101	−0.118	−437	−579
E7: $(5p4f^2)_{11/2}^o$	0.46	0.52	1.187	1.184	0.091	0.079	307	274
E8: $(5p4f^2)_{5/2}^o$	0.02	0.08	1.152	1.188	0.079	0.085	502	581
E9: $(5p4f^2)_{13/2}^o$	0.13	0.12	1.144	1.149	−0.040	−0.009	−748	−703

**Table 4.** The static scalar and tensor electric dipole polarizabilities,  $\alpha_S^{E1}$  and  $\alpha_T^{E1}$  (in a.u.), the magnetic dipole polarizabilities,  $\alpha^{M1}$  (in a.u.), the values of the reduced matrix elements of  $\langle J||T^{(2)}||J \rangle$  (in a.u.), and the coefficient of the relativistic sensitivity  $K$  to variations in  $\alpha$ .

Items	G0: $(5p^24f)_{5/2}^o$	G1: $(5p^24f)_{7/2}^o$	E0: $(5p4f^2)_{9/2}^o$
$\alpha_S^{E1}(J)$	2.218	2.220	2.235
$\alpha_T^{E1}(J)$	−0.04	−0.06	0.01
$\alpha^{M1}(J)$	−4.62	3.45	−2.12
$\alpha^{M1}(F, M_F)=(3,2)$	$−1.53 \times 10^5$	$−1.28 \times 10^6$	$−1.12 \times 10^5$
$\langle J  T^{(2)}  J \rangle$	−73.67	−85.23	−85.20
$K$		0.72	6.52

### 5. Conclusions

In conclusion, we investigated the atomic structure of the  $\text{Nd}^{9+}$  ion as a possible clock frequency standard. Many spectroscopic properties, such as energy levels, lifetimes,  $g_j$  factors, electric quadrupole moments, electric dipole polarizabilities, and magnetic-dipole hyperfine structure constants of the low-lying atomic states, were provided by using comparative computations based on the MRCI and CI+MBPT methods. The dominant systematics in  $\text{Nd}^{9+}$  are attainable below the level of  $10^{-19}$ . Moreover, a strong sensitivity to violation of the Lorentz invariance and variations in the fine-structure constant  $\alpha$  was

found in Nd<sup>9+</sup>. All of these findings strongly suggest the aptness of the Nd<sup>9+</sup> ion as a promising optical clock and cast its great potential for application for the probing of new physics beyond the Standard Model.

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## References

1. Windberger, A.; López-Urrutia, J.C.; Bekker, H.; Oreshkina, N.S.; Berengut, J.C.; Bock, V.; Versolato, O.O. Identification of the Predicted 5s-4f Level Crossing Optical Lines with Applications to Metrology and Searches for the Variation of Fundamental Constants. *Phys. Rev. Lett.* **2015**, *114*, 150801. [[CrossRef](#)] [[PubMed](#)]
2. Nakajima, T.; Okada, K.; Wadac, M.; Dzuba, V.A.; Safronova, M.S.; Safronova, U.I.; Ohmae, N.; Katori, H.; Nakamura, N. Visible spectra of highly charged holmium ions observed with a compact electron beam ion trap. *Nucl. Instrum. Methods Phys. Res. B* **2017**, *408*, 118. [[CrossRef](#)]
3. Bekker, H.; Borschevsky, A.; Harman, Z.; Keitel, C.H.; Pfeifer, T.; Schmidt, P.O.; López-Urrutia, J.R.C.; Berengut, J.C. Detection of the 5p-4f orbital crossing and its optical clock transition in Pr<sup>9+</sup>. *Nat. Commun.* **2019**, *10*, 5651. [[CrossRef](#)] [[PubMed](#)]
4. Liang, S.Y.; Zhang, T.X.; Guan, H.; Lu, Q.F.; Xiao, J.; Chen, S.L.; Huang, Y.; Zhang, Y.H.; Li, C.B.; Zou, Y.M.; et al. Probing multiple electric-dipole-forbidden optical transitions in highly charged nickel ions. *Phys. Rev. A* **2021**, *103*, 022804. [[CrossRef](#)]
5. Micke, P.; Leopold, T.; King, S.A.; Benkler, E.; Spiess, L.J.; Schmoger, L.; Schwarz, M.; Lopez-Urrutia, J.R.C.; Schmidt, P.O. Coherent laser spectroscopy of highly charged ions using quantum logic. *Nature* **2020**, *578*, 60. [[CrossRef](#)] [[PubMed](#)]
6. Berengut, J.C.; Dzuba, V.A.; Flambaum, V.V.; Ong, A. Highly charged ions with E1, M1, and E2 transitions within laser range. *Phys. Rev. A* **2012**, *86*, 022517. [[CrossRef](#)]
7. Olsen, J.; Jørgensen, P.; Simons, J. Passing The Onebillion Limit In Full Configuration-Interaction (FCI) Calculations. *Chem. Phys. Lett.* **1990**, *169*, 463. [[CrossRef](#)]
8. Fleig, T.; Olsen, J.; Visscher, L. The generalized active space concept for the relativistic treatment of electron correlation. II. Large-scale configuration interaction implementation based on relativistic 2- and 4-spinors and its application. *J. Chem. Phys.* **2003**, *119*, 2963. [[CrossRef](#)]
9. Fleig, T.; Jensen, H.J.A.; Olsen, J.; Visscher, L. The generalized active space concept for the relativistic treatment of electron correlation. III. Large-scale configuration interaction and multiconfiguration self-consistent-field fourcomponent methods with application to UO<sub>2</sub>. *J. Chem. Phys.* **2006**, *124*, 104106. [[CrossRef](#)] [[PubMed](#)]
10. Dzuba, V.A.; Flambaum, V.V.; Kozlov, M.G. Combination of the many-body perturbation theory with the configuration-interaction method. *Phys. Rev. A* **1996**, *54*, 3948. [[CrossRef](#)] [[PubMed](#)]
11. Kahl, E.V.; Berengut, J.C. ambit: A programme for high-precision relativistic atomic structure calculations. *Computer Phys. Comm.* **2019**, *238*, 232. [[CrossRef](#)]
12. Gomes, A.S.P.; Dyal, K.G.; Visscher, L. Relativistic double-zeta, triple-zeta, and quadruple-zeta basis sets for the lanthanides La-Lu. *Theor. Chem. Acc.* **2010**, *127*, 369. [[CrossRef](#)]
13. Gomes, A.S.P.; Saue, T.; Visscher, L.; Jensen, H.J.A.; Bast, R.; Aucar, W.C.F.I.A.; Bakken, V.; Dyal, K.G.; Dubillard, S.; Ekström, U.; et al. DIRAC, a Relativistic ab Initio Electronic Structure Program, Release DIRAC19. 2019. Available online: <http://www.diracprogram.org> (accessed on 1 February 2019).
14. Flambaum, V.V.; Ginges, J.S.M. Radiative potential and calculations of QED radiative corrections to energy levels and electromagnetic amplitudes in many-electron atoms. *Phys. Rev. A* **2005**, *72*, 052115. [[CrossRef](#)]
15. Huo, X.; Jiang, G.; Li, X. Atomic properties and transition parameters of highly charged Sb-like isoelectronic ions. *Can. J. Phys.* **2017**, *95*, 594. [[CrossRef](#)]