# Atomic Structure Calculations for Pb$^{+70}$ and Pb$^{+71}$

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This paper describes a detailed theoretical analysis of energies, Landé $g$-factors, lifetimes for excited levels, and wavelengths, transition probabilities, and weighted oscillator strengths for electric dipole transitions for Mg- and Na-like lead. Recently, the accurate atomic knowledge of highly ionized heavy atoms has been attractive for many fields, such as laser physics and astrophysics. We used two independent atomic codes to determine atomic data. These are a Hartree–Fock code including superposition of configurations with relativistic corrections, and AUTOSTRUCTURE code which includes Breit interactions and quantum electrodynamics contributions. The calculated data were compared graphically with available works in order to confirm the reliability of our results. In general, we reached a good agreement. The obtained new atomic data for Pb ions were not reported before. This study provides a reference for analyzing astrophysical spectra.

topics: relativistic corrections, wavelengths, oscillator strengths, transition probabilities

## 1. Introduction

In recent years, there has been considerable interest in the research on highly ionized high-Z elements. Accurate atomic data for these ions are necessary not only for atomic physics but also for many fields of science and technology, such as plasma physics, laser physics, astrophysics, fusion applications, etc. Heavy elements are used in fusion environments, and their spectra supply important information on plasma parameters [1–3]. On the other hand, Na-like ions with a valance electron and Mg-like ions with two valence electrons out of a closed core are convenient systems for theoretical calculations.

In the past few years, some calculations have been employed to determine atomic data about Mg-like ions. These data have been studied following various relativistic approaches. But there is a lack of complete energy levels and transition data for upper levels of Mg-like Pb (Pb$^{+70}$, $Z = 82$). Recently, Hu et al. [4] calculated the $n = 3$ to $n' = 3$ transitions using multiconfiguration Dirac–Hartree–Fock (MCDHF) and relativistic configuration interaction (RCI) method in the Mg isoelectronic sequence of Pb. Santana and Träbert [5, 6] reported the relativistic multi-reference Møller–Plesset (MR–MP) many-body perturbation theory calculations for $3s3p$, $3p^2$, $3s3d$, $3p3d$, and $3d^2$ levels in Mg-like Pb. Energy levels and electric dipole (E1), electric

quadrupole (E2), magnetic dipole (M1), and magnetic quadrupole (M2) transition parameters were presented by employing the fully relativistic model-potential Flexible Atomic Code (FAC) by Iorga and Stancalie [7].

For Na-like Pb (Pb$^{+71}$, $Z = 82$) ion, there is no detailed data for energy levels and transition parameters in the literature. Seely and Wagner [8] reported quantum electrodynamics (QED) contributions to the $3s$–$3p$ transitions in highly charged Na-like ions. Resonance transition energies of Na-like ions were presented by Kim et al. [9]. E1, E2, and M1 transition probabilities among states with principal quantum numbers $n = 3$ and $4$ were computed using Dirac–Fock single–configuration wave functions for Na-like Pb ion by Baik et al. [10]. Blundell [11] calculated the screened self-energy and vacuum polarization in Na-like ions. Beiersdorfer and Wargelin [12] made a measurement of the $3s_{1/2}$–$3p_{3/2}$ transition energies in Na-like Pb. Simionovici et al. [13] reported on $n = 3$ to $n' = 3$ soft-X-ray transitions for Na-like Pb. Johnson et al. [14] presented transition probabilities for Na-like ions. Transition energies of the D lines in Na-like ions were investigated by Gillaspy et al. [15]. Sapirstein and Cheng performed $S$-matrix calculations of energy levels of Na-like ions [16]. Relativistic distorted-wave collision strengths and oscillator strengths for $\Delta n = 0$ transitions in Na-like ions were computed by Fontes and Zhang [17].

In this study, a consistent data set of energy levels, Landé $g$-factors, lifetimes, wavelengths, weighted oscillator strengths, and transition probabilities for E1 transitions are reported for Mg-like Pb (Pb$^{+70}$, $Z = 82$) and Na-like Pb (Pb$^{+71}$, $Z = 82$). Na-like ions are essential to the diagnostics of fusion energy devices [18] and in astronomy [19]. Also, Mg-like ions are highly useful in the characterization of astrophysical and laboratory plasmas based on temperature and electron density [20, 21]. The ground state configuration for Pb$^{70+}$ and Pb$^{71+}$ ions are [Ne]$3s^2$ and [Ne]$3s$, respectively. The AUTOSTRUCTURE (AUTOS.) and pseudo-relativistic Hartree–Fock (HFR) atomic codes have been used for the calculations. The HFR method considers the correlation effects and relativistic corrections. The AUTOSTRUCTURE results include contributions of QED (i.e., self–energy and vacuum polarization) and Breit interaction (magnetic interaction between the electrons and retardation effects of the electron–electron interaction), as well as correlation effects (valence–valence (VV), core–valence (CV), and core–core (CC)), which are significant for investigations involving the electronic structure and spectroscopic properties of many-electron systems. In addition, the electron correlation effects due to the Coulomb interaction between the electrons are also important, particularly on fine structure and transitions.

## 2. Calculation method

The AUTOSTRUCTURE code developed by Badnell [22] and the pseudo-relativistic Hartree–Fock method developed by Cowan (Cowan's HFR method) [23] have been used in the calculations.

The theoretical basis of these methods was described in detail in [24, 25] and was applied successfully in previous works by our working group [26, 27]. So we only briefly summarize it here.

In HFR and AUTOSTRUCTURE, wave functions are calculated with the Breit–Pauli relativistic corrections. This Hamiltonian can be written as

$$H_{\mathrm{BP}} = H_{\mathrm{NR}} + H_{\mathrm{RC}}, \qquad (1)$$

where $H_{\mathrm{NR}}$ is the usual nonrelativistic Hamiltonian

$$H_{\mathrm{NR}} = \sum_{i=1}^{N} h(i) + \sum_{j>i=1}^{N} \frac{1}{r_{ij}} =$$

$$\sum_{i=1}^{N} \left( -\frac{1}{2}\nabla_i^2 - \frac{Z}{r_i} \right) + \sum_{j>i=1}^{N} \frac{1}{r_{ij}}, \qquad (2)$$

and $H_{\mathrm{RC}}$ contains the relativistic correction operators, which include one-body relativistic operators (spin–orbit interaction, the non-fine-structure mass variation, and the one-body Darwin corrections) and two-body Breit operators (spin–other–orbit, the mutual spin–spin, the spin–spin contact, the two-body Darwin, and the orbit–orbit terms). Unlike in AUTOSTRUCTURE, two-body operators are neglected in HFR Hamiltonian.

In AUTOSTRUCTURE atomic code, the probability for spontaneous emission by electric dipole (E1) radiation is

$$A_{i' \to i} = 2.6774 \times 10^9 \frac{(E_i - E_{i'})}{g_i} S(i, i'), \qquad (3)$$

where $g_i$ is statistically weighted of level, $E_i$ and $E_{i'}$ are energies of levels, and $S(i, i')$ is line strength in the form

$$S(i, i') = \left| \left\langle i' \left\| R^{[k]} \right\| i \right\rangle \right|^2, \qquad (4)$$

where $R^{[k]}$ is a transition operator and describes each multipole, and $k$ is 1 for electric dipole radiation.

The weighted absorption or emission oscillator strength $(gf)$ value can be written in terms of line strength

$$(gf)_{i,i'} = (gf)_{i',i} = \frac{|E_i - E_{i'}|}{3} S(i, i'). \qquad (5)$$

According to the HFR method, the total electric dipole (E1) transition probability from a state $\gamma' J' M'$ to all states $M$ levels of $\gamma J$ is given by

$$A_{E1} = \frac{64\pi^4 e^2 a_0^2 \sigma^3}{3h(2J'+1)} \boldsymbol{S} \qquad (6)$$

and absorption oscillator strength is given by

$$f_{ij} = \frac{2(E_j - E_i)}{3(2J+1)} \boldsymbol{S}, \qquad (7)$$

where $\boldsymbol{S}$ is the electric dipole line strength

$$\boldsymbol{S} = \left| \left\langle \gamma J \left\| \boldsymbol{P}^{(1)} \right\| \gamma' J' \right\rangle \right|^2 \qquad (8)$$

in atomic units of $e^2 a_0^2$ and $\sigma = [(E_j - E_i)/hc]$ has units of kaysers [cm$^{-1}$].

Most experiments yield the lifetime of the upper level because of easy measuring. In this case, the sum over multipole transitions to all lower-lying levels must be taken. The lifetime $\tau$ for a level j is defined as follows

$$\tau_j = \frac{1}{\sum_i A_{ji}}. \qquad (9)$$

## 3. Results and discussion

Herein, we have calculated the energies, Landé $g$-factors, lifetimes, and radiative parameters such as wavelengths ($\lambda$ [Å]), weighted oscillator strengths ($gf$), and transition probabilities ($A_{ji}$ [s$^{-1}$]) for electric dipole (E1) transitions in Mg-like Pb (Pb $^{70+}$) and Na-like Pb (Pb$^{71+}$) using AUTOSTRUCTURE [22] and HFR codes [23]. The results of this work are given in Tables I–III and Figs. 1–10, where they are compared with available data. In the tables, the odd-parity states are indicated by the superscript "$o$", and we have omitted the filled subshells $1s^2 2s^2 2p^6$ neon core. References to values from other sources are given below the tables with a superscript lowercase letter. Also, the new results of this work are presented in Tables SI and SII in the supplementary material [28].

TABLE I

Energies ($E$), Landé $g$-factors, and lifetimes ($\tau$) of $3l3l'$ ($l, l' = 0, 1, 2$) levels for Pb$^{+70}$. Numbers in brackets represent powers of 10.

| No. | Levels | | $E$ [cm$^{-1}$] | | | | | $g$-factors | $\tau$ [ps] |
|---|---|---|---|---|---|---|---|---|---|
| | | | This work | | Other works | | | This work | This work |
| | | | AUTOS. | HFR | MR–MP[a] | MCDHF[b] | FAC[c] | HFR | HFR |
| 1 | $3s^2$ | $^1S_0$ | 0 | 0 | 0 | 0 | 0 | 0.00 | – |
| 2 | $3s3p$ | $^3P_0^o$ | 1343818 | 1200873 | 1334575 | 1331878.95 | 1375895.00 | 0.00 | 4.81(1) |
| 3 | $3s3p$ | $^3P_1^o$ | 1500378 | 1353251 | 1482132 | 1479906.43 | 1529201.67 | 1.35 | – |
| 4 | $3p^2$ | $^3P_0$ | 3200074 | 2901703 | 3169969 | 3166216.05 | 3274475.00 | 0.00 | 7.16 |
| 5 | $3s3p$ | $^3P_2^o$ | 6217690 | 6404664 | 6202117 | 6207723.27 | 6411120.83 | 1.50 | – |
| 6 | $3s3p$ | $^1P_1^o$ | 6560248 | 6733537 | 6540902 | 6547518.69 | 6763793.33 | 1.15 | 1.41(−1) |
| 7 | $3p^2$ | $^1D_2$ | 7911664 | 7929577 | 7880116 | 7881581.37 | 8142199.17 | 1.14 | 1.70 |
| 8 | $3p^2$ | $^3P_1$ | 7938150 | 7974678 | 7905770 | 7909397.39 | 8171566.67 | 1.50 | 1.88(−1) |
| 9 | $3s3d$ | $^3D_1$ | 8173869 | 8099180 | 8167706 | 8166791.60 | 8440541.67 | 0.50 | 2.42(−1) |
| 10 | $3s3d$ | $^3D_2$ | 8322194 | 8263856 | 8304962 | 8306724.29 | 8585741.67 | 1.15 | 1.19(−1) |
| 11 | $3s3d$ | $^3D_3$ | 9301419 | 9249595 | 9247132 | 9247166.97 | 9553800.00 | 1.33 | 2.98 |
| 12 | $3s3d$ | $^1D_2$ | 9460716 | 9398671 | 9400531 | 9402006.50 | 9714791.67 | 1.06 | 1.41 |
| 13 | $3p3d$ | $^3F_2^o$ | 9620348 | 9423204 | 9601282 | 9598047.72 | 9917333.33 | 0.76 | 1.92(1) |
| 14 | $3p3d$ | $^3D_1^o$ | 9940094 | 9710509 | 9924305 | 9922234.43 | 10254616.67 | 0.83 | 1.80(−1) |
| 15 | $3p3d$ | $^3P_2^o$ | 10918203 | 10722091 | 10857093 | 10855019.19 | 11214358.33 | 1.29 | 2.58 |
| 16 | $3p3d$ | $^1F_3^o$ | 10960933 | 10758213 | 10888930 | 10887409.72 | 11248058.33 | 1.11 | 3.59 |
| 17 | $3p^2$ | $^3P_2$ | 12873296 | 13233776 | 12834575 | 12846829.49 | 13270550.00 | 1.33 | 9.74(−2) |
| 18 | $3p^2$ | $^1S_0$ | 13048548 | 13401802 | 13013624 | 13026622.64 | 13457616.67 | 0.00 | 9.95(−2) |
| 19 | $3p3d$ | $^3D_2^o$ | 14611831 | 14727677 | 14593954 | 14599119.26 | 15083000.00 | 1.05 | 1.10(−1) |
| 20 | $3p3d$ | $^3P_0^o$ | 14695356 | 14803921 | 14685641 | 14691012.56 | 15178183.33 | 0.00 | 1.07(−1) |
| 21 | $3p3d$ | $^3P_1^o$ | 14702882 | 14821044 | 14689103 | 14694527.52 | 15178758.33 | 1.10 | 1.08(−1) |
| 22 | $3p3d$ | $^3F_3^o$ | 14712004 | 14822909 | 14684532 | 14690569.04 | 15182291.67 | 1.09 | 1.17(−1) |
| 23 | $3p3d$ | $^3F_4^o$ | 15637580 | 15762455 | 15568121 | 15574212.72 | 16086716.67 | 1.25 | 2.13(−1) |
| 24 | $3p3d$ | $^1D_2^o$ | 15734312 | 15868709 | 15673256 | 15679392.33 | 16196116.67 | 1.23 | 1.86(−1) |
| 25 | $3p3d$ | $^3D_3^o$ | 15907442 | 16044103 | 15837129 | 15844243.02 | 16367533.33 | 1.22 | 1.84(−1) |
| 26 | $3p3d$ | $^1P_1^o$ | 16015680 | 16149968 | 15954199 | 15962150.72 | 16489983.33 | 1.07 | 1.71(−1) |
| 27 | $3d^2$ | $^3F_2$ | 16463366 | 16330756 | 16465337 | 16464114.86 | 17017616.67 | 0.78 | 1.25(−1) |
| 28 | $3d^2$ | $^3P_0$ | 16698417 | 16556452 | 16713272 | 16713454.77 | 17277975.00 | 0.00 | 1.15(−1) |
| 29 | $3d^2$ | $^3F_3$ | 17553252 | 17439206 | 17505641 | 17505051.37 | 18088658.33 | 1.08 | 2.35(−1) |
| 30 | $3d^2$ | $^3P_2$ | 17652457 | 17542820 | 17614691 | 17614585.22 | 18203216.67 | 1.17 | 2.18(−1) |
| 31 | $3d^2$ | $^1G_4$ | 17701661 | 17576267 | 17636804 | 17637361.77 | 18226100.00 | 1.06 | 2.58(−1) |
| 32 | $3d^2$ | $^3P_1$ | 17698190 | 17580539 | 17667324 | 17667137.19 | 18258183.33 | 1.50 | 2.13(−1) |
| 33 | $3d^2$ | $^3F_4$ | 18726421 | 18627708 | 18625763 | 18626536.64 | 19243775.00 | 1.19 | 1.70 |
| 34 | $3d^2$ | $^1D_2$ | 18808471 | 18714370 | 18723513 | 18724644.26 | 19346483.33 | 1.21 | 1.38 |
| 35 | $3d^2$ | $^1S_0$ | 19059722 | 18951604 | 18980213 | 18983704.87 | 19616808.33 | 0.00 | 9.91(−1) |

[a] Ref. [6], [b]Ref. [4], [c]Ref. [7]

### 3.1. Mg-like Pb

In our AUTOSTRUCTURE calculation, we have included valance–valance, core–valance, and core–core correlations and the configurations: $3lnl'$ ($l = 0$-$2$, $n = 3$-$6$, $l, = 0$-$4$), $2p^53s^23l$ ($l = 1$-$2$), $2p^53s3p^2$, $2p^53p^3$, $2p^53s^24s$, $2p^53s3p3d$, $2p^53p^23d$, $2p^53s3p4s$, $2p^53l3d^2$ ($l = 0$-$2$), $2p^53p3d4s$, $2s2p^53s^23p3d$, $2p^43s3p^3$, $2p^43s^23l3l'$ ($l = 1$-$2$, $l' = 1$-$2$).

For HFR calculation, we have taken into account only the configurations including one electron excitation from valence to other subshells: $3s^2$, $3p^2$, $3d^2$, $3snd$ ($n = 3$-$8$), $3sns$ ($n = 4$-$8$), $3sng$ ($n = 5$-$8$), $3sni$ ($n = 7, 8$), $3pnp$ ($n = 4$-$8$), $3pnf$ ($n = 4$-$8$), $3pnh$ ($n = 6$-$8$), $3snp$ ($n = 3$-$8$), $3snf$ ($n = 4$-$8$), $3snh$ ($n = 6$-$8$), $3pnd$ ($n = 3$-$8$), $3pnd$ ($n = 3$-$8$), $3pns$ ($n = 4$-$8$), $3pns$ ($n = 4$-$8$), $3png$ ($n = 5$-$8$). In the calculation, the Hamiltonian's calculated eigenvalues were not optimized to the observed energy
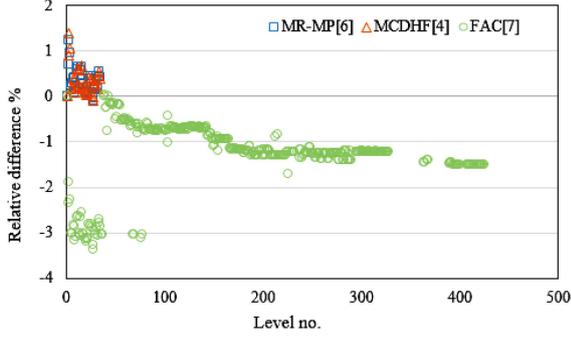
Fig. 1. The percentage differences between the present energies (AUTOSTRUCTURE) and other theoretical results for Mg-like Pb [4, 6, 7].
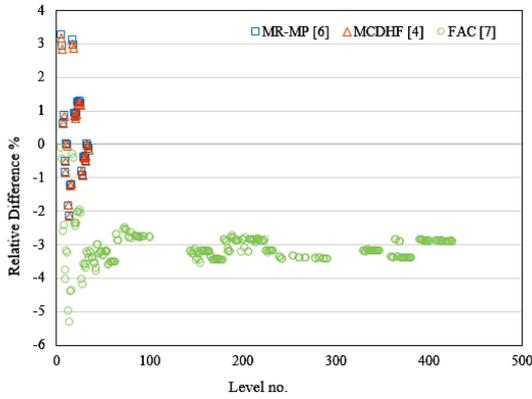


Fig. 2. The percentage differences between the present energies (HFR) and other theoretical results for Mg-like Pb [4, 6, 7].



Fig. 3. Comparison of the present $\log(S)$ calculated in this work (AUTOSTRUCTURE) with those of Hu et al. [4] for E1 transitions of Mg-like Pb.
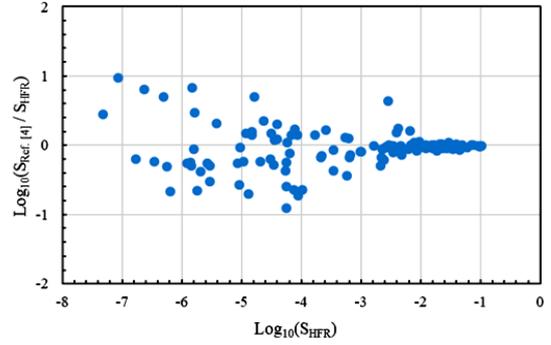


Fig. 4. Comparison of the present $\log(S)$ calculated in this work (HFR) with those of Hu et al. [4] for E1 transitions of Mg-like Pb.

levels via a least–squares fitting ($LSF$) procedure using experimentally determined energy levels. That was because experimentally determined energy levels are not available in the literature for $Pb^{+70}$. The scaling factors of the Slater parameters ($F^k$ and $G^k$) and configuration interaction integrals ($R^k$) that were not optimized in $LSF$, were chosen as 0.95 for calculation, while the spin-orbit parameters were left at their initial values. The calculated HFR results are reported as *ab initio* results (Tables I–III, SI–SII).

In Table I, we have listed only the energy levels, Landé $g$-factors, and lifetimes ($\tau$) of $3l3l'$ ($l, l' = 0, 1, 2$) levels for $Pb^{+70}$. The energy levels are relative to the $3s^2\ {}^1S_0$ ground state. As can be seen in Table I, the results obtained from the AUTOS. and HFR calculations are in agreement with the results obtained from MR–MP [6], MCDHF [4], and FAC [7]. We have calculated the differences in percent (($(|E_{\text{present}} - E_{\text{others}}|/E_{\text{others}}) \times 100$) to assess the accuracy of our results for all levels. The percent differences between AUTOS. results from our and other works [4, 6, 7] are in the range of 0.01–3.35%. When the differences between our HFR results and theoretical data of [4, 6, 7] are in

the range of 0.01–5.30% (except for the $3s3p\ {}^3P^o_{0,1}$ and $3p^2\ {}^3P_0$ levels, where the differences are up to 8.35–12.73%). We have also graphically compared our results with the results obtained from MR–MP [6], MCDHF [4], and FAC [7] for all levels. The percentage of the relative differences (($(E_{\text{present}} - E_{\text{others}})/E_{\text{others}}\%$) with the MR–MP, MCDHF, and FAC results is illustrated in Figs. 1 and 2. Figure 2 does not include the energies values of $3s3p\ {}^3P^o_{0,1}$ and $3p^2\ {}^3P_0$ levels. As seen in these figures, the energy results obtained from our calculations are in agreement with the available results.

Weighted oscillator strengths ($gf$) and transition probabilities ($A_{ij}$ [s$^{-1}$]) for E1 transitions between the levels of $3l3l'$ ($l, l' = 0, 1, 2$) in $Pb^{+70}$ are graphically compared (Figs. 3–7). Figures 3 and 4 show $\log_{10}(S_{\text{OW}}/S_{\text{TW}})$ as a function of line strength $\log_{10}(S_{\text{TW}})$ for E1 transitions in, respectively, AUTOSTRUCTURE and HFR calculations. Using the uncertainty estimation method suggested by Kramida [29, 30], we estimated the uncertainties of $S$-values for E1 transitions using an estimator $dS = \log_{10}(S_{\text{OW}}/S_{\text{TW}})$, where OW means other work and TW means this work. Here, we refer to the
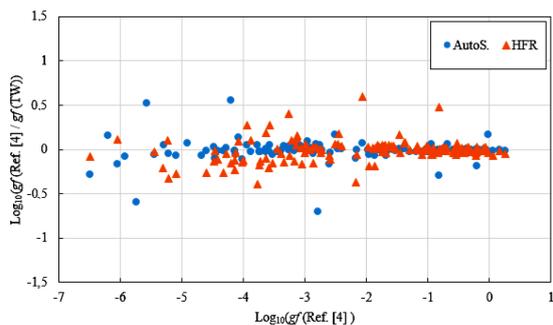
Fig. 5.  Comparison of the present $\log(gf)$ calculated in this work (TW: AUTOSTRUCTURE and HFR) with those of Hu et al. [4] for E1 transitions of Mg-like Pb.



Fig. 6.  Comparison of the present $\log_{10}(A_{ij})$ calculated in this work (TW: AUTOSTRUCTURE and HFR) with those of Hu et al. [4] for E1 transitions of Mg-like Pb.
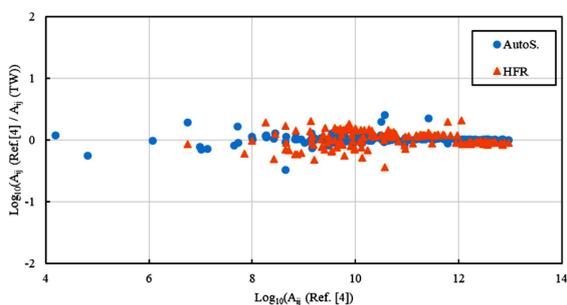


Fig. 7.  Comparison of the present $\log_{10}(A_{ij})$ calculated in this work (TW: AUTOSTRUCTURE and HFR) with those of Iorga et al. [7] for E1 transitions of Mg-like Pb.

results given in [4] and compared to our AUTOS. and HFR results. The root mean square (rms) of d$S$ is equal to $\sqrt{\mathrm{d}S^2}$, and percentage uncertainty is estimated as $u\% = (10^{\mathrm{rms}} - 1) \times 100$. According to Figs. 3 and 4, if few outliers are excluded, the agreement between $\log_{10}(S_{\mathrm{OW}})$ and $\log_{10}(S_{\mathrm{TW}})$ for the E1 transitions with $(\log_{10} S_{\mathrm{TW}} \geq -2.17)$ is 8.5% for AUTOS. and 7.7% for HFR.

The $gf$ computed in the present work $(\log(gf)$ (AUTOS.) and $\log(gf)$ (HFR)) for the E1 transitions between the levels of $3l3l'$ $(l, l' = 0, 1, 2)$ in Pb$^{+70}$ are compared with the available results from [4] in Fig. 5. The comparison shows that our results agree with those of [4]. If these few outliers are excluded, the rms value of $\log_{10}(gf)$ $([4])/(gf)$ (AUTOS.) for these transitions is 0.111. This corresponds to an average difference of about 29%. For HFR calculation, the rms value (0.097) of the relative differences reaches 25%, from [4], except for some transitions. Also, the comparison of the transitions between our transition probabilities ($A_{ij}$) and MCDHF [4] (calculation B) and FAC results [7] has been displayed in Figs. 6 and 7. As seen in Figs. 6 and 7, our transition probabilities agree with [4] and [7], except for some transitions. The rms value of the relative differences between our results and other works has been found in the val-

ues 19% and 26% for the comparison of AUTOS. with [4, 7] and 33% and 31% for the comparison of HFR with [4, 7], respectively, except for some transitions. The agreement between the presented data is strong evidence for the reliability of the HFR and AUTOS. calculations for $gf$ and $A_{ij}$.

### 3.2. Na-like Pb

We have considered the $nl$ $(n = 3$–$6$, $l = 0$–$5)$, $2p^5 3snl$ $(n = 3$–$5$, $l = 0$–$4)$, $2p^5 3pnl$ $(n = 3$–$5$, $l = 0$–$4)$, $2p^5 3dnl$ $(n = 3$–$5$, $l = 0$–$4)$, $2p^4 3s^2 3p$, $2p^4 3s^2 3d$, $2s2p^5 3s^2 3p$ configurations in AUTOSTRUCTURE calculation and the $nl$ $(n = 3$–$15$, $l = 0$–$6)$ configurations in the HFR calculation. These configurations have been considered for correlation effects (including VV, CV, and CC correlations in AUTOSTRUCTURE and VV correlation in HFR). According to the configurations mentioned, we have obtained 1630 energy levels for AUTOSTRUCTURE and 149 energy levels for HFR.

In HFR calculation, the Hamiltonian's calculated eigenvalues were optimized to the observed energy levels via a least-squares fitting (LSF) procedure using experimentally determined energy levels, specifically the two levels from [12]. The scaling factors of the Slater parameters ($F^k$ and $G^k$) and configuration interaction integrals ($R^k$), not optimized in the least-squares fitting, were chosen as 0.95 for calculation, while the spin-orbit parameters were left at their initial values.

Table II gives the energies, Landé $g$-factors, and lifetimes of $nl$ $(n \leq 6, l \leq 5)$ levels for Pb$^{+71}$. The energy levels are relative to the $3s$ $^2\mathrm{S}_{1/2}$ ground state. References for other comparison values are typed with a superscript lowercase letter. There are only $3l$ and $4l$ levels for this ion in the literature for comparison. As can be seen in Table II, our results are in agreement with other works. We have calculated the mean ratio (AUTOSTRUCTURE/HFR) for the accuracy of our results. The mean ratio of energy levels for our HFR and AUTOS. calculations is 1.02. The agreement between the presented data is strong evidence for the reliability of the HFR

TABLE II

Energies ($E$), Landé $g$-factors, and lifetimes ($\tau$) of $nl$ ($n \leq 6$, $l \leq 5$) levels for Pb$^{+71}$. Numbers in brackets represent powers of 10.

| No. | Levels | | $E$ [cm$^{-1}$] | | | $g$-factors | $\tau$ [ps] |
|---|---|---|---|---|---|---|---|
| | | | This work | | Other works | This work | This work |
| | Conf. | Term | AUTOS. | HFR | | HFR | HFR |
| 1 | $3s$ | $^2S_{1/2}$ | 0 | 0 | 0 | 2.00 | |
| 2 | $3p$ | $^2P^o_{1/2}$ | 1531666 | 1518510 | 1526564.76[a] | 0.67 | 1.67(1) |
| | | | | | 1519049[b] | | |
| | | | | | 1518695[c] | | |
| | | | | | 1518499.22[d] | | |
| | | | | | 1518511.8[e] | | |
| | | | | | 1518015.28[g] | | |
| | | | | | 1506569[h] | | |
| | | | | | 1549447.37[i] | | |
| 3 | $3p$ | $^2P^o_{3/2}$ | 6449362 | 6442050 | 6448399.23[a] | 1.33 | 2.19(−1) |
| | | | | | 644008[b] | | |
| | | | | | 6445375[c] | | |
| | | | | | 6442430.73[d] | | |
| | | | | | 6442541.5[e] | | |
| | | | | | 6442053.7[f] | | |
| | | | | | 6442430.73[g] | | |
| | | | | | 6429044[h] | | |
| | | | | | 6443127.58[i] | | |
| 4 | $3d$ | $^2D_{3/2}$ | 8145982 | 8087830 | 8167972.36[a] | 0.80 | 2.77(−1) |
| | | | | | 8142811[h] | | |
| 5 | $3d$ | $^2D_{5/2}$ | 9292945 | 9253130 | 9263272.69[a] | 1.20 | 2.96 |
| | | | | | 9241948[h] | | |
| 6 | $4s$ | $^2S_{1/2}$ | 34299810 | 33761050 | 33743224[h] | 2.00 | 8.24(−3) |
| 7 | $4p$ | $^2P^o_{1/2}$ | 34868176 | 34313330 | 34361919[h] | 0.67 | 1.18(−2) |
| 8 | $4p$ | $^2P^o_{3/2}$ | 36940192 | 36481360 | 36378593[h] | 1.33 | 9.81(−3) |
| 9 | $4d$ | $^2D_{3/2}$ | 37588305 | 37025510 | 37028326[h] | 0.80 | 4.22(−3) |
| 10 | $4d$ | $^2D_{5/2}$ | 38088391 | 37522830 | 37503102[h] | 1.20 | 5.93(−3) |
| 11 | $4f$ | $^2F^o_{5/2}$ | 38423299 | 37852510 | 37836122[h] | 0.86 | 2.41(−3) |
| 12 | $4f$ | $^2F^o_{7/2}$ | 38636524 | 38066530 | 38045817[h] | 1.14 | 2.64(−3) |
| 13 | $5s$ | $^2S_{1/2}$ | 49299019 | 48747650 | – | 2.00 | 1.08(−2) |
| 14 | $5p$ | $^2P^o_{1/2}$ | 49628877 | 49021180 | – | 0.67 | 1.38(−2) |
| 15 | $5p$ | $^2P^o_{3/2}$ | 50642356 | 50113930 | – | 1.33 | 1.25(−2) |
| 16 | $5d$ | $^2D_{3/2}$ | 50943313 | 50379920 | – | 0.80 | 6.14(−3) |
| 17 | $5d$ | $^2D_{5/2}$ | 51200551 | 50635190 | – | 1.20 | 8.04(−3) |
| 18 | $5f$ | $^2F^o_{5/2}$ | 51364737 | 50798940 | – | 0.86 | 4.70(−3) |
| 19 | $5f$ | $^2F^o_{7/2}$ | 51474829 | 50909260 | – | 1.14 | 5.06(−3) |
| 20 | $5g$ | $^2G_{7/2}$ | 51496672 | 50930510 | – | 0.89 | 8.43(−3) |
| 21 | $5g$ | $^2G_{9/2}$ | 51561172 | 50994810 | – | 1.11 | 8.71(−3) |
| 22 | $6s$ | $^2S_{1/2}$ | 58341822 | 56673250 | – | 2.00 | 1.57(−2) |
| 23 | $6p$ | $^2P^o_{1/2}$ | 58551381 | 56826800 | – | 0.67 | 1.90(−2) |
| 24 | $6p$ | $^2P^o_{3/2}$ | 59117679 | 57452130 | – | 1.33 | 1.78(−2) |
| 25 | $6d$ | $^2D_{3/2}$ | 59279145 | 57602150 | – | 0.80 | 9.44(−3) |
| 26 | $6d$ | $^2D_{5/2}$ | 59427640 | 57749880 | – | 1.20 | 1.19(−2) |

TABLE II cont.

| No. | Levels | | $E$ [cm$^{-1}$] | | | $g$-factors | $\tau$ [ps] |
| | | | This work | | Other works | This work | This work |
| | Conf. | Term | AUTOS. | HFR | | HFR | HFR |
|---|---|---|---|---|---|---|---|
| 27 | $6f$ | $^2F^o_{7/2}$ | 59519547 | 57842910 | – | 0.86 | 8.09(−3) |
| 28 | $6f$ | $^2F^o_{7/2}$ | 59583983 | 57906960 | – | 1.14 | 8.61(−3) |
| 29 | $6g$ | $^2G_{7/2}$ | 59597377 | 57921010 | – | 0.89 | 1.46(−2) |
| 30 | $6g$ | $^2G_{9/2}$ | 59634820 | 57958360 | – | 1.11 | 1.50(−2) |
| 31 | $6h$ | $^2H^o_{9/2}$ | 59635186 | 57959520 | – | 0.91 | 2.22(−2) |
| 32 | $6h$ | $^2H^o_{11/2}$ | 59659933 | 57984160 | – | 1.09 | 2.26(−2) |

[a]Ref. [17], [b]Ref. [9], [c]Ref. [8], [d]Ref. [11], [e]Ref. [15], [f]Ref. [12], [g]Ref. [16], [h]Ref. [10], [i]Ref. [14]
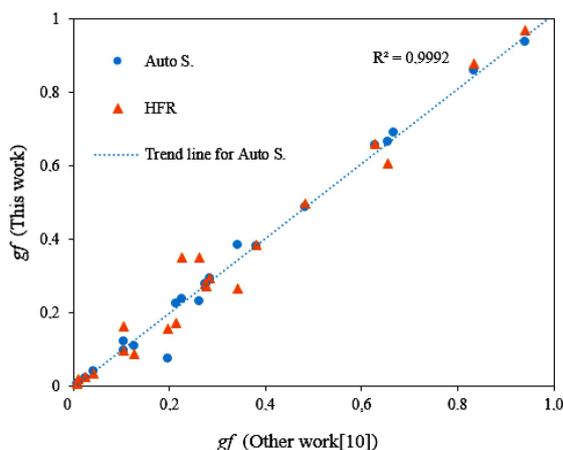


Fig. 8. Comparison of the weighted oscillator strengths calculated in this work (AUTOSTRUC-TURE and HFR) with those of Baik et al. [10] for E1 transitions of Na-like Pb.
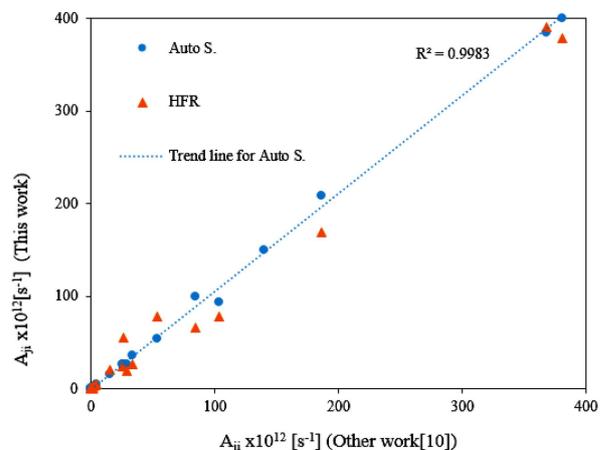


Fig. 9. Comparison of the transition probabilities calculated in this work (AUTOSTRUCTURE and HFR) with those of Baik et al. [10] for E1 transitions of Na-like Pb.

and AUTOS. calculations. Also, the energies, Landé $g$-factors, and lifetimes of upper levels, which are new results, are given in the supplementary material in Table SI [28] for HFR calculation.

We have obtained 339316 and 2296 possible E1 transitions for the selected configurations in the AUTOS. and HFR calculations, respectively. Transition probabilities ($A_{ji}$ [s$^{-1}$]), weighted oscillator strengths ($gf$), wavelengths ($\lambda$ [Å]), and line strengths ($S$ [a. u.]) for E1 transitions between the levels of $3l$ ($l = 0, 1, 2$) and $4l$ ($l = 0, 1, 2, 3$) are listed in Table III. In this table, the number in brackets represents the power of 10. Our results are in good agreement with other works [8–10, 14, 17], as seen in Table III. We have calculated the mean ratio $gf$ (this work)/ $gf$ (other work) for the accuracy of our results. The mean ratio between our results and other works [10] has been found in the values 0.99 and 1.07 for AUTOS. and HFR calculations, respectively. As seen in Table III, the results obtained from the AUTOS. and HFR calculations are in agreement with other works within transition probabilities results. We have found the
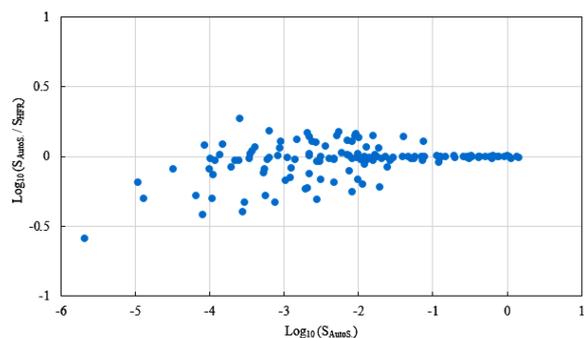


Fig. 10. Comparison of line strengths derived in this work from the AUTOSTRUCTURE calculations with the HFR calculations for E1 transitions of Na-like Pb.

values 1.02 and 1.07 for the mean ratio of $A_{ji}$ (this work)/$A_{ji}$ [10], respectively. Also, $gf$ and $A_{ji}$ comparisons of the E1 transitions have been presented in, respectively, Figs. 8 and 9 (except the transition 2.82 Å (in HFR)).

Transition probabilities ($A_{ji}$), weighted oscillator strengths ($gf$), and wavelengths ($\lambda$) for electric dipole (E1) transitions between the levels of $3l$ ($l = 0, 1, 2$) and $4l$ ($l = 0, 1, 2, 3$) in Pb$^{+71}$. Numbers in brackets represent powers of 10.

| Transitions | | | | Method | $A_{ji}$ [s$^{-1}$] | | $gf$ | | $\lambda$ [Å] | | $S$ [a. u.] |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Upper level | | Lower level | | | This work | Other works | This work | Other works | This work | Other works | This work |
| $3p$ | $^2P^o_{1/2}$ | $3s$ | $^2S_{1/2}$ | AUTOS. | 5.75(10) | 3.515(10)[a] | 7.35(−2) | 7.02(−2)[b] | 65.29 | 65.854[d] | 1.58(−2) |
| | | | | HFR | 5.98(10) | 5.375(10)[b] | 7.77(−2) | 7.1142(−2)[c] | 65.85 | 65.846[e] | 1.69(−2) |
| $3p$ | $^2P^o_{3/2}$ | $3s$ | $^2S_{1/2}$ | AUTOS. | 4.56(12) | 4.569(12)[a] | 6.57(−1) | 6.628(−1)[a] | 15.51 | 15.5218[d] | 1.68(−2) |
| | | | | HFR | 4.56(12) | 4.545(12)[b] | 6.59(−1) | 6.6484(−1)[c] | 15.52 | 15.515[e] | 1.68(−2) |
| $3d$ | $^2D_{3/2}$ | $3p$ | $^2P^o_{1/2}$ | AUTOS. | 3.55(12) | 3.542(12)[a] | 4.87(−1) | 4.822(−1)[a] | 15.12 | – | 1.21(−2) |
| | | | | HFR | 3.95(12) | | 4.99(−1) | 4.8272(−1)[c] | 15.22 | | 1.37(−2) |
| $3d$ | $^2D_{3/2}$ | $3p$ | $^2P^o_{3/2}$ | AUTOS. | 1.17(10) | 1.204(10)[a] | 2.43(−2) | 2.458(−2)[a] | 58.94 | – | 4.73(−3) |
| | | | | HFR | 1.13(10) | | 2.50(−2) | 2.4672(−2)[c] | 60.76 | | 5.00(−3) |
| $3d$ | $^2D_{5/2}$ | $3p$ | $^2P^o_{3/2}$ | AUTOS. | 3.43(11) | 3.355(11)[a] | 3.82(−1) | 3.814(−1)[a] | 35.17 | – | 2.95(−2) |
| | | | | HFR | 3.38(11) | | 3.84(−1) | 3.8162(−1)[c] | 35.57 | | 3.00(−2) |
| $4s$ | $^2S_{1/2}$ | $3p$ | $^2P^o_{1/2}$ | AUTOS. | 2.71(13) | 2.663(13)[a] | 7.55(−2) | 1.968(−1)[a] | 3.05 | – | 0.76(−3) |
| | | | | HFR | 5.48(13) | 2.767(13)[b] | 1.58(−1) | | 3.10 | | 1.61(−3) |
| $4s$ | $^2S_{1/2}$ | $3p$ | $^2P^o_{3/2}$ | AUTOS. | 9.95(13) | 8.486(13)[a] | 3.85(−1) | 3.410(−1)[a] | 3.59 | – | 9.09(−3) |
| | | | | HFR | 6.66(13) | 8.594(13)[b] | 2.68(−1) | | 3.66 | | 6.45(−3) |
| $4p$ | $^2P^o_{1/2}$ | $3s$ | $^2S_{1/2}$ | AUTOS. | 9.42(13) | 1.034(14)[a] | 2.32(−1) | 2.626(−1)[a] | 2.87 | – | 2.20(−3) |
| | | | | HFR | 7.80(13) | | 3.51(−1) | | 2.74 | | 1.58(−3) |
| $4p$ | $^2P^o_{1/2}$ | $3d$ | $^2D_{3/2}$ | AUTOS. | 2.65(13) | 2.922(13)[a] | 1.11(−1) | 1.274(−1)[a] | 3.74 | – | 2.74(−3) |
| | | | | HFR | 2.00(13) | | 8.73(−2) | | 3.81 | | 2.18(−3) |
| $4p$ | $^2P^o_{1/2}$ | $4s$ | $^2S_{1/2}$ | AUTOS. | 1.05(10) | 1.325(12)[a] | 9.76(−2) | 1.038(−1)[a] | 175.94 | – | 5.64(−2) |
| | | | | HFR | 1.00(10) | | 9.83(−2) | | 181.07 | | 5.86(−2) |
| $4p$ | $^2P^o_{3/2}$ | $3s$ | $^2S_{1/2}$ | AUTOS. | 5.43(13) | 5.388(13)[a] | 2.39(−1) | 2.258(−1)[a] | 2.71 | – | 1.07(−3) |
| | | | | HFR | 7.80(13) | | 3.51(−1) | | 2.74 | | 1.58(−3) |
| $4p$ | $^2P^o_{3/2}$ | $3d$ | $^2D_{3/2}$ | AUTOS. | 1.33(12) | 1.428(12)[a] | 9.63(−3) | 1.074(−2)[a] | 3.47 | – | 1.10(−4) |
| | | | | HFR | 2.54(12) | | 1.89(−2) | | 3.52 | | 2.19(−4) |
| $4p$ | $^2P^o_{3/2}$ | $3d$ | $^2D_{5/2}$ | AUTOS. | 1.59(13) | 1.551(13)[a] | 1.24(−1) | 1.052(−1)[a] | 3.62 | – | 2.23(−3) |
| | | | | HFR | 2.02(13) | | 1.63(−1) | | 3.67 | | 2.96(−3) |
| $4p$ | $^2P^o_{3/2}$ | $4s$ | $^2S_{1/2}$ | AUTOS. | 1.09(12) | 1.090(12)[a] | 9.37(−1) | 9.416(−1)[a] | 37.87 | – | 5.84(−2) |
| | | | | HFR | 1.20(12) | | 9.69(−1) | | 36.76 | | 5.88(−2) |
| $4d$ | $^2D_{3/2}$ | $3p$ | $^2P^o_{1/2}$ | AUTOS. | 1.50(14) | 1.400(14)[a] | 6.90(−1) | 6.656(−1)[a] | 2.77 | – | 3.15(−3) |
| | | | | HFR | 2.09(14) | | 9.96(−1) | | 2.82 | | 4.63(−3) |
| $4d$ | $^2D_{3/2}$ | $3p$ | $^2P^o_{3/2}$ | AUTOS. | 3.65(13) | 3,320(13)[a] | 2.26(−1) | 2.126(−1)[a] | 3.21 | – | 2.38(−3) |
| | | | | HFR | 2.68(13) | | 1.72(−1) | | 3.27 | | 1.85(−3) |
| $4d$ | $^2D_{3/2}$ | $4p$ | $^2P^o_{1/2}$ | AUTOS. | 1.06(12) | 9.878(11)[a] | 8.59(−1) | 8.332(−1)[a] | 36.76 | – | 5.20(−2) |
| | | | | HFR | 1.08(12) | | 8.78(−1) | | 36.87 | | 5.34(−2) |
| $4d$ | $^2D_{3/2}$ | $4p$ | $^2P^o_{3/2}$ | AUTOS. | 2.85(9) | 2.863(9)[a] | 4.07(−2) | 4.064(−2)[a] | 154.29 | – | 2.07(−2) |
| | | | | HFR | 1.74(9) | | 3.53(−2) | | 183.77 | | 2.13(−2) |
| $4d$ | $^2D_{5/2}$ | $3p$ | $^2P^o_{3/2}$ | AUTOS. | 2.09(14) | 1.862(14)[a] | 1.87(0) | 1.734(0)[a] | 3.16 | – | 1.30(−2) |
| | | | | HFR | 1.69(14) | | 1.57(0) | | 3.22 | | 1.11(−2) |
| $4d$ | $^2D_{5/2}$ | $4p$ | $^2P^o_{3/2}$ | AUTOS. | 9.76(10) | 9.208(10)[a] | 6.66(−1) | 6.550(−1)[a] | 87.09 | – | 1.27(−1) |
| | | | | HFR | 7.32(10) | | 6.07(−1) | | 96.02 | | 1.28(−1) |
| $4f$ | $^2F^o_{5/2}$ | $3d$ | $^2D_{3/2}$ | AUTOS. | 3.85(14) | 3.682(14)[a] | 3.78(0) | 3.756(0)[a] | 3.30 | – | 2.73(−2) |
| | | | | HFR | 3.90(14) | | 3.96(0) | | 3.36 | | 2.92(−2) |
| $4f$ | $^2F^o_{5/2}$ | $3d$ | $^2D_{5/2}$ | AUTOS. | 2.63(13) | 2.511(13)[a] | 2.79(−1) | 2.762(−1)[a] | 3.43 | – | 3.14(−3) |
| | | | | HFR | 2.47(13) | | 2.72(−1) | | 3.50 | | 3.14(−3) |
| $4f$ | $^2F^o_{5/2}$ | $4d$ | $^2D_{3/2}$ | AUTOS. | 2.30(10) | 2.066(10)[a] | 2.96(−1) | 2.848(−1)[a] | 119.76 | – | 7.80(−2) |
| | | | | HFR | 2.25(10) | | 2.96(−1) | | 120.92 | | 7.85(−2) |

TABLE III cont.

| Transitions | | | | Method | $A_{ji}$ [s$^{-1}$] | | $gf$ | | $\lambda$ [Å] | | $S$ [a. u.] |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Upper level | | Lower level | | | This work | Other works | This work | Other works | This work | Other works | This work |
| $4f$ | $^2F^o_{5/2}$ | $4d$ | $^2D_{5/2}$ | AUTOS. | 1.04(8) | 1.015(8)$^a$ | 8.32(−3) | 8.232(−3)$^a$ | 298.59 | – | 8.20(−3) |
| | | | | HFR | 1.02(8) | | 8.42(−3) | | 303.32 | | 8.43(−3) |
| $4f$ | $^2F^o_{7/2}$ | $3d$ | $^2D_{5/2}$ | AUTOS. | 4.00(14) | 3.807(14)$^a$ | 5.58(0) | 5.503(0)$^a$ | 3.41 | – | 4.70(−2) |
| | | | | HFR | 3.79(14) | | 5.48(0) | | 3.47 | | 4.69(−2) |
| $4f$ | $^2F^o_{7/2}$ | $4d$ | $^2D_{5/2}$ | AUTOS. | 6.95(9) | 6.740(9)$^a$ | 2.78(−1) | 2.744(−1)$^a$ | 182.44 | – | 1.25(−1) |
| | | | | HFR | 6.84(9) | | 2.78(−1) | | 183.93 | | 1.26(−1) |

$^a$Ref. [10], $^b$Ref. [14], $^c$Ref. [18], $^d$Ref. [17], $^e$Ref. [9]

Transition data for E1 transitions from principal quantum numbers $n = 5$ and $n = 6$ to lower levels are given in the supplementary material in Table SII [28]. These values for these transitions have been presented for the first time. The mean ratio of transition probabilities and weighted oscillator strengths for all our HFR and AUTOS. calculations (Table III and Table SII) are 1.01 and 1.00, respectively, except for the transition $6s\ ^2S_{1/2}-3p\ ^2P^o_{1/2}$. Also, the line strengths derived from these AUTOS. calculations ($\log_{10}(S_{AUTOS.})$) were compared with the HFR calculation ($\log_{10}(S_{HFR})$) for our results in Table III and Table SII. The rms value of $\log_{10}(S_{AUTOS.}/S_{HFR})$ for 78 transitions out of a total of 138 depicted in Fig. 10 is 0.015. This corresponds to a reasonable difference of about 3.5%.

## 4. Conclusion

In summary, we have performed HFR and AUTOSTRUCTURE calculations for Pb$^{+70}$ and Pb$^{+71}$. In the presented work, new energies, the Landé $g$-factors, lifetimes for excited levels, and electric dipole parameters such as transition probabilities, wavelengths, and weighted oscillator strengths are reported in the tables. Also, comparisons with available works have been made graphically as well. The compared results have a good agreement, in general. We believe that our present work may help fill the gap and provide high-accuracy data for highly-ionized heavy ions that are significant for fusion plasma research and astrophysics.

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