# Multiconfiguration Dirac-Fock Energy Level and Radiative Rates for E1, E2, M1 and M2 Transition in Hf LXIII, Ta LXIV, W LV and Re LXVI

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## Abstract

**In Present Paper, we have reported multiconfiguration Dirac-Fock transition energies and wavefunction compositions of 209 levels belonging to the configurations$2s^22p^6$, $2s^22p^5ns$ (n=3,4,5,6,7), $2s^22p^5np$ (n=3,4,5,6,7), $2s^22p^5nd$ (n=3,4,5,6,7), $2s^22p^5nf$ (n=4,5), $2s^22p^55g$, $2s2p^6ns$(n=3,4,5), $2s2p^6np$ (n=3,4,5), $2s2p^6nd$ (n=3,4,5), $2s2p^6nf$ (n=4,5) and $2s2p^65g$ of Hf LXIII, Ta LXIV, W XV and Re LXVI. Radiative rates, oscillator strengths, transition wavelengths and line strengths have been calculated for all electric dipole (E1), magnetic dipole (M1), electric quadrupole (E2) and magnetic quadrupole (M2) transitions among these levels. These values were obtained using the GRASP (general-purpose relativistic atomic structure package) code which includes Breit and QED effects along with Dirac-Fock potential and second order coulomb interaction. We have compared our results with the data complied using FAC (Flexible Atomic Code) and also with the recent results available in the literature. The accuracy of the data is assessed. We predict new energy levels, oscillator strength and transition probability data, where no other theoretical or experimental results are available, which will form the basis for future experimental work.**

## Introduction

**In recent years, study of Ne-like ions remains of interest as spectra of these ions are the source of many important diagnostics informations on plasma such as electron temperature, electron density and charge state abundance. Ne-like ions of middle and high atomic number are present in tokamak, laser produced plasma, EBIT, solar atmosphere [1-4]. Also, Ne-like ions are highly useful for the modelling of astrophysical, fusion and laser generated plasma. Further, because of their closed shell structure, we can estimate the importance of the contributions from relativistic, electron correlations and quantum electrodynamics (QED) effects in study of energy values and radiative rates particularly, transitions between levels of $2p^53s$, 3p and 3d configurations produce prominent lines in the spectra of high temperature light source in Ne-like ions . To obtain laser action the 3s and 3p states have utilized. Also, laser is obtained in lighter elements for Ne-like ions . Therefore, we have studied atomic data of Ne-like ions for Z=72-75.**

**Table1. MCDF energies (in Ryd.), lifetimes (in s) and mixing coefficients in Ne-like- W**

| S.No | Label | J | Level (Ryd) | FAC | NIST | Ref. [24] | Lifetimes | Mixing coefficients |
|---|---|---|---|---|---|---|---|---|
| 1 | $2s^22p^{6}\,^1S^e$ | 0 | ---------- | 0 | 0 | 0.0000 | ---------- | 100 |
| 2 | $2s^22p^53s\ ^3P^o$ | 2 | 609.646919 | 609.7976 | | 609.6024 | 2.31E-10 | 100 |
| 3 | $2s^22p^53s\ ^1P^o$ | 1 | 610.267422 | 610.4177 | 610.6401 | 610.2292 | 6.48E-15 | 66.26+33.76(19) |
| 4 | $2s^22p^53p\ ^3P^e$ | 1 | 620.748586 | 620.7565 | | 620.6689 | 1.53E-11 | 49.42+31.58(25) |
| 5 | $2s^22p^53p\ ^3D^e$ | 2 | 620.877261 | 620.8838 | | 620.7976 | 1.04E-12 | 50.27+33.29(24)+16.48(8) |
| 6 | $2s^22p^53p\ ^1P^e$ | 1 | 648.608985 | 648.636 | | 648.5388 | 6.28E-13 | 55.95+36(25) |
| 7 | $2s^22p^53p\ ^3D^e$ | 3 | 648.575977 | 648.6648 | | 648.5082 | 6.00E-13 | 100 |
| 8 | $2s^22p^53p\ ^3P^e$ | 2 | 649.54187 | 649.591 | | 649.4658 | 3.72E-13 | 66.75+33.29(24) |
| 9 | $2s^22p^53p\ ^1S^e$ | 0 | 653.837013 | 653.808 | 653.8587 | 653.7288 | 4.08E-13 | 62.25+37.7(21) |
| 10 | $2s^22p^53d\ ^3P^o$ | 0 | 660.298438 | 660.2802 | | 660.2404 | 8.19E-13 | 100 |
| 11 | $2s^22p^53d\ ^3P^o$ | 1 | 661.03207 | 661.0127 | 661.507 | 660.9754 | 1.21E-14 | 66.1+23.26(29) |
| 12 | $2s^22p^53d\ ^3F^o$ | 3 | 661.09547 | 661.0764 | | 661.0420 | 7.79E-13 | 53.88+39.19(31) |
| 13 | $2s^22p^53d\ ^3D^o$ | 2 | 661.693976 | 661.6689 | | 661.6386 | 7.43E-13 | 54.46+18.32(28)+17.56(15) |
| 14 | $2s^22p^53d\ ^3F^o$ | 4 | 667.199226 | 667.2074 | | 667.1448 | 6.41E-12 | 100 |
| 15 | $2s^22p^53d\ ^1D^o$ | 2 | 667.7274 | 667.7173 | | 667.6732 | 3.52E-12 | 48.44+41.09(30) |
| 16 | $2s^22p^53d\ ^3D^o$ | 3 | 668.470303 | 668.4545 | | 668.4160 | 5.85E-12 | 70.56+27.25(31) |
| 17 | $2s^22p^53d\ ^1P^o$ | 1 | 670.649232 | 670.5868 | 670.246 | 670.5722 | 3.59E-16 | 62.88+18.75(29)+18.23(11) |
| 18 | $2s^22p^53s\ ^3P^o$ | 0 | 711.476523 | 711.721 | | 711.4577 | 3.16E-11 | 99.8 |
| 19 | $2s^22p^53s\ ^3P^o$ | 1 | 711.723347 | 711.9678 | 711.936 | 711.7088 | 2.56E-14 | 66.26+33.76(3) |
| 20 | $2s^22p^53p\ ^3D^e$ | 1 | 722.283258 | 722.3909 | | 722.2374 | 1.52E-11 | 73.62+22.66(6) |
| 21 | $2s^22p^53p\ ^3P^e$ | 0 | 725.916062 | 725.9919 | 726.088 | 725.8494 | 3.01E-12 | 62.25+37.58(9) |
| 22 | $2s2p^63s\ ^3S^e$ | 1 | 747.074015 | 746.9027 | | 746.8320 | 5.64E-14 | 85.01 |
| 23 | $2s2p^63s\ ^1S^e$ | 0 | 750.437584 | 750.0166 | | 750.0804 | 4.64E-14 | 99.8 |
| 24 | $2s^22p^53p\ ^1D^e$ | 2 | 750.730625 | 750.8837 | | 750.6897 | 3.55E-13 | 49.7+33.52(24)+16.81(8) |
| 25 | $2s^22p^53p\ ^3S^e$ | 1 | 751.427697 | 751.4487 | | 751.3483 | 1.27E-13 | 42.51+25.4(25) |
| 26 | $2s2p^63p\ ^3P^o$ | 0 | 759.093117 | 758.5398 | | 758.8086 | 4.37E-14 | 99.8 |
| 27 | $2s2p^63p\ ^3P^o$ | 1 | 758.914026 | 758.6759 | 758.302 | 758.6382 | 1.22E-15 | 65.93+31.81(33) |
| 28 | $2s^22p^53d\ ^3F^o$ | 2 | 762.889496 | 762.98 | | 762.8610 | 7.44E-13 | 74.3+20.43(15) |
| 29 | $2s^22p^53d\ ^3D^o$ | 1 | 764.890545 | 764.8985 | 765.027 | 764.8414 | 7.53E-16 | 47.61+34.57(17) |
| 30 | $2s^22p^53d\ ^3P^o$ | 2 | 769.496164 | 769.5792 | | 769.4660 | 3.36E-12 | 46.92+36.12(13) |
| 31 | $2s^22p^53d\ ^1F^o$ | 3 | 769.747452 | 769.8329 | | 769.7196 | 5.23E-12 | 43.96+33.52(31)+22.47(16) |
| 32 | $2s2p^63p\ ^3P^o$ | 2 | 787.066016 | 786.7087 | | 786.8023 | 4.06E-14 | 99.6 |
| 33 | $2s2p^63p\ ^1P^o$ | 1 | 787.508545 | 787.1479 | 786.651 | 787.2457 | 2.13E-15 | 67.73+32.15(27) |

**Table 2: Transition wavelength (in Å), transition probability in $s^{-1}$, oscillator strength (dimensionless), line strength (length form) for E1 transition using MCDF for Ne-like W**

| i | j | λ (in Å) | $A_{ji}(s^{-1})$ | $f_{ij}$ | $S_{ij}$(au) | Vel./len. |
|---|---|---|---|---|---|---|
| $2s^22p^{61}S_0$ | $2s^22p^53s\ ^1P_1$ | 1.49E+00 | 1.54E+14 | 1.55E-01 | 7.60E-04 | 9.90E-01 |
| $2s^22p^{61}S_0$ | $2s^22p^53d\ ^3P_1$ | 1.38E+00 | 8.14E+13 | 6.96E-02 | 3.16E-04 | 1.00E+00 |
| $2s^22p^{61}S_0$ | $2s^22p^53d\ ^1P_1$ | 1.36E+00 | 2.79E+15 | 2.31E+00 | 1.04E-02 | 1.00E+00 |
| $2s^22p^{61}S_0$ | $2s^22p^53s\ ^3P_1$ | 1.28E+00 | 3.90E+13 | 2.88E-02 | 1.21E-04 | 9.70E-01 |
| $2s^22p^{61}S_0$ | $2s2p^63p\ ^3P_1$ | 1.20E+00 | 7.99E+14 | 5.18E-01 | 2.05E-03 | 1.00E+00 |
| $2s^22p^{61}S_0$ | $2s^22p^53d\ ^3D_1$ | 1.19E+00 | 1.33E+15 | 8.46E-01 | 3.32E-03 | 1.00E+00 |
| $2s^22p^{61}S_0$ | $2s2p^63p\ ^1P_1$ | 1.16E+00 | 4.46E+14 | 2.68E-01 | 1. 02E-03 | 1.00E+00 |
| $2s^22p^{61}S_0$ | $2s^22p^54s\ ^1P_1$ | 1.07E+00 | 5.44E+13 | 2.79E-02 | 9.78E-05 | 9.50E-01 |
| $2s^22p^{61}S_0$ | $2s^22p^54d\ ^3P_1$ | 1.04E+00 | 3.24E+13 | 1.58E-02 | 5.43E-05 | 9.90E-01 |
| $2s^22p^{61}S_0$ | $2s^22p^54d\ ^1P_1$ | 1.04E+00 | 1.01E+15 | 4.87E-01 | 1.66E-03 | 9.90E-01 |
| $2s^22p^{61}S_0$ | $2s^22p^54s\ ^3P_1$ | 9.53E-01 | 1.96E+13 | 8.01E-03 | 2.51E-05 | 9.10E-01 |
| $2s^22p^{61}S_0$ | $2s^22p^55s\ ^1P_1$ | 9.46E-01 | 3.21E+13 | 1.29E-02 | 4.03E-05 | 9.10E-01 |
| $2s^22p^{61}S_0$ | $2s^22p^55d\ ^3P_1$ | 9.36E-01 | 2.08E+13 | 8.21E-03 | 2.53E-05 | 9.90E-01 |
| $2s^22p^{61}S_0$ | $2s^22p^55d\ ^1P_1$ | 9.34E-01 | 2.29E+14 | 8.99E-02 | 2.77E-04 | 9.80E-01 |
| $2s^22p^{61}S_0$ | $2s^22p^54d\ ^3D_1$ | 9.32E-01 | 8.88E+14 | 3.47E-01 | 1.07E-03 | 9.90E-01 |
| $2s^22p^{61}S_0$ | $2s2p^64p\ ^3P_1$ | 9.14E-01 | 1.44E+14 | 5.40E-02 | 1.63E-04 | 9.80E-01 |
| $2s^22p^{61}S_0$ | $2s2p^64p\ ^1P_1$ | 9.04E-01 | 2.38E+14 | 8.74E-02 | 2.60E-04 | 9.80E-01 |
| $2s^22p^{61}S_0$ | $2s^22p^56s\ ^1P_1$ | 8.93E-01 | 1.48E+13 | 5.30E-03 | 1.56E-05 | 8.40E-01 |
| $2s^22p^{61}S_0$ | $2s^22p^56d\ ^3P_1$ | 8.87E-01 | 9.38E+12 | 3.32E-03 | 9.71E-06 | 9.70E-01 |
| $2s^22p^{61}S_0$ | $2s^22p^56d\ ^1P_1$ | 8.86E-01 | 2.63E+14 | 9.29E-02 | 2.71E-04 | 9.70E-01 |
| $2s^22p^{61}S_0$ | $2s^22p^57s\ ^1P_1$ | 8.64E-01 | 8.04E+12 | 2.70E-03 | 7.67E-06 | 1.00E+00 |
| $2s^22p^{61}S_0$ | $2s^22p^57d\ ^3P_1$ | 8.61E-01 | 5.89E+12 | 1.96E-03 | 5.56E-06 | 1.00E+00 |
| $2s^22p^{61}S_0$ | $2s^22p^57d\ ^1P_1$ | 8.60E-01 | 1.50E+14 | 4.97E-02 | 1.41E-04 | 1.00E+00 |
| $2s^22p^{61}S_0$ | $2s^22p^55s\ ^3P_1$ | 8.56E-01 | 8.84E+12 | 2.91E-03 | 8.20E-06 | 8.30E-01 |
| $2s^22p^{61}S_0$ | $2s^22p^55d\ ^3D_1$ | 8.47E-01 | 3.18E+14 | 1.03E-01 | 2.86E-04 | 9.80E-01 |
| $2s^22p^{61}S_0$ | $2s2p^65p\ ^3P_1$ | 8.26E-01 | 7.89E+13 | 2.42E-02 | 6.59E-05 | 9.80E-01 |
| $2s^22p^{61}S_0$ | $2s2p^65p\ ^1P_1$ | 8.22E-01 | 1.33E+14 | 4.03E-02 | 1.09E-04 | 9.60E-01 |
| $2s^22p^{61}S_0$ | $2s^22p^56s\ ^3P_1$ | 8.11E-01 | 5.13E+12 | 1.52E-03 | 4.06E-06 | 7.60E-01 |
| $2s^22p^{61}S_0$ | $2s^22p^56d\ ^3D_1$ | 8.07E-01 | 1.68E+14 | 4.92E-02 | 1.31E-04 | 9.60E-01 |
| $2s^22p^{61}S_0$ | $2s^22p^57s\ ^3P_1$ | 7.87E-01 | 2.79E+12 | 7.78E-04 | 2.02E-06 | 9.30E-01 |
| $2s^22p^{61}S_0$ | $2s^22p^57d\ ^3D_1$ | 7.85E-01 | 9.90E+13 | 2.74E-02 | 7.08E-05 | 1.00E+00 |

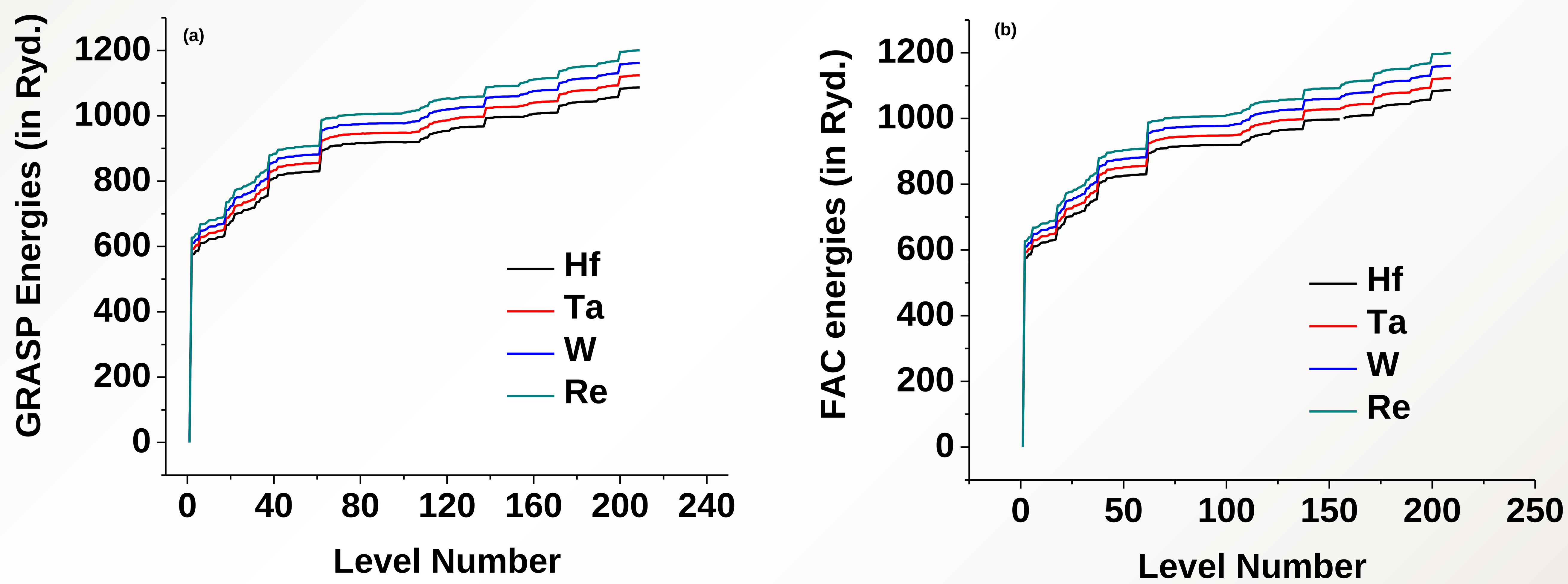


**Figure 1. (a) GRASP energies (b) FAC energies in Ryd. for 209 levels of Ne-like ions**

**1. From figures (a) and (b), we observe that energies of Ne-like Hf to W ions for lowest levels are very close.**

**2. For levels greater than 5, energies increases very rapidly.**

**3. Energy of a particular level for higher nuclear charge Ne-like ion is larger as compared low nuclear charge Ne-like ions.**

**4. Difference between energies of Ne-like ions increases as we go from lower level to higher level.**

**5. Energy levels calculated from GRASP and FAC are good in agreement with each other for Ne-like ions.**

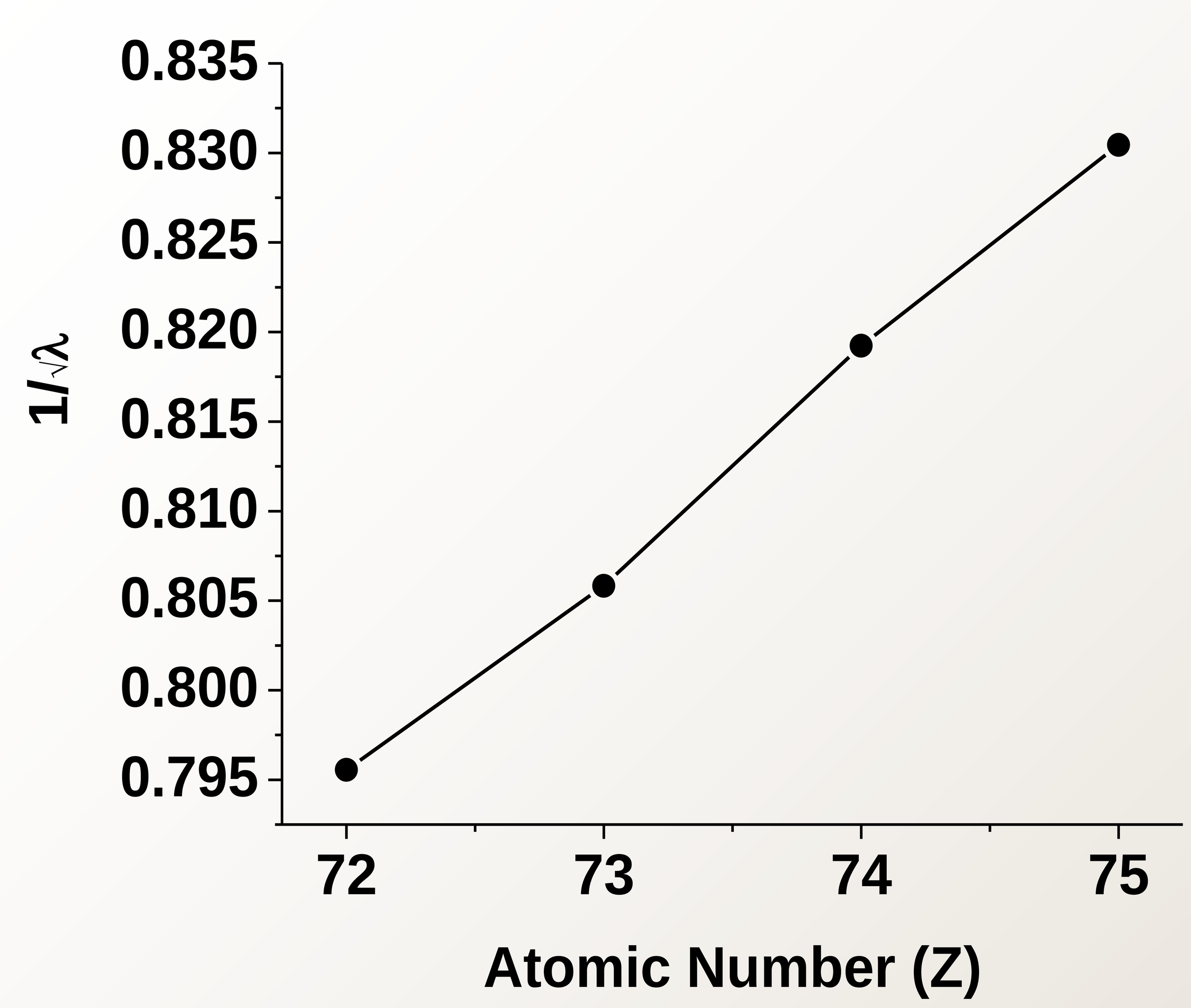


**Figure 2. Trend of 1/ √λ (in $10^5\ m^{-1}$) with atomic number Z for Lα transition $2s^22p^6\ ^1S_0^e - 2s^22p^53s\ ^1P_1^o$**

1. **In Fig. 2, by using slope-intercept formula, we have calculated Mosley's parameters K and σ, where σ is screening constant. K= 0.0118103 and σ = 4.6815322**
2. **By using the above parameters, one can easily calculate the transition wavelength for this transition for any Ne-like ion.**
3. **The similar process can be applied for other X-ray transitions of Ne-like ions.**

## Conclusion

1. Our calculated results from FAC and GRASP are in good agreement with each other and matches well with NIST.
2. The trend of transition wavelengths with nuclear charge follows Mosley's law for L-alpha transitions in Ne-like ions .
3. The presented results may be beneficial in fusion and astrophysical plasma applications .

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