Comment on “Energy levels and radiative rates for Ne-like ions from Cu to Ga” by N. Singh and S. Aggarwal [Pramana – J. Phys. 89 (2017) 79]

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Abstract

Recently, N. Singh and S. Aggarwal [Pramana – J. Phys. 89 (2017) 79] have reported energies and lifetimes for 127 levels of three Ne-like ions, namely Cu XX, Zn XXI and Ga XXII. For the calculations they have adopted two independent atomic structure codes, i.e. GRASP and FAC, and have concluded that both codes give comparable energies. However, we find that the differences between the two sets of energies are up to 1.5 Ryd (over $1.6 \times 10^5$ wavenumbers) for many levels, and for all three ions. In the absence of other available theoretical or experimental data, it becomes difficult to know which set of energies is more accurate. Through our calculations with the same code we demonstrate that their listings from the FAC calculations are incorrect. A few more anomalies noted in their tabulated results are also highlighted.
1 Introduction

In a recent paper, Singh and Aggarwal [1] have reported results for energy levels, radiative rates (A-values), and lifetimes ($\tau$) among 127 levels of three Ne-like ions, namely Cu XX, Zn XXI and Ga XXII. These levels belong to the $2s^22p^6$, $2s^22p^53\ell$, $2s2p^63\ell$, $2s^22p^54\ell$, $2s2p^64\ell$ and $2s^22p^55\ell$ ($\ell \leq 3$) configurations. For the calculations, they have adopted two independent atomic structure codes, i.e. the general-purpose relativistic atomic structure package (GRASP) and the flexible atomic code (FAC), which are available at the websites http://amdpp.phys.strath.ac.uk/UKAPAP/codes.html and https://www-amdis.iaea.org/FAC/, respectively. It was done for the assessment of accuracy, particularly for the energy levels, because prior similar data, experimental or theoretical, for most of the levels for these three ions do not exist. Therefore, based on the two calculations they concluded that both codes provide ‘comparable energies’. However, we notice that for many levels of all three ions the differences between the two sets of energies are significant, i.e. up to 1.5 Ryd – see for example, levels 111–127 of Cu XX, 112–119 of Zn XXI and 111-116 of Ga XXII in their tables 1–3. In our long experience for a wide range of ions we have not noticed such large differences between calculations with these two codes, particularly when the same level of CI (configuration interaction) has been used. Additionally, in the absence of any other similar data, it is difficult to know which set of energies is more accurate. Therefore, we have performed our own calculations with these two codes and note that while their energies with the GRASP are correct, with FAC are not.

2 Energy levels

In both calculations (with GRASP and FAC) Singh and Aggarwal [1] have included CI among 51 configurations, namely $2s^22p^6$, $2s^22p^5n\ell$ ($3 \leq n \leq 7$, but $\ell \leq 3$), $2s2p^6n\ell$ ($3 \leq n \leq 7$, but $\ell \leq 3$), $2s^22p^43\ell3\ell'$ and $2s^22p^43\ell3\ell'$. These configurations generate 1016 levels in total, but the results have been reported for only among 127, as noted in Section 1. Since both codes are fully relativistic and the same CI has been used in both calculations, the results obtained are expected to be comparable, and this has also been concluded by them. However, some of the energies obtained between the two calculations differ by up to $\sim$1.5 Ryd as noted already, and therefore their conclusion is not based on the calculated data. Since such discrepancies unnecessarily confuse the users of data, we have performed our own calculations with both codes, and with the same CI. Their listed energies obtained with GRASP are found to be comparable with our own calculations, but not with FAC. We discuss these in detail below.

In tables 1–3 we list our calculated energies with FAC along with those of Singh and Aggarwal [1] for 127 levels of Cu XX, Zn XXI and Ga XXII. Only their final energies, obtained with the inclusion of Breit and quantum electrodynamic effects (QED), are listed in these tables, but with both the GRASP and the FAC. Two conclusions can be easily drawn from these tables. Firstly, there are no appreciable differences between the GRASP and FAC2 (our calculations) energies for any of the ion considered here. This result is fully expected and has been noted in the past for several other ions. Secondly, and more importantly, there are significant differences between the GRASP and FAC1 energies obtained by Singh and Aggarwal. Differences in FAC1 and FAC2 energies for the lowest about 100 levels of these ions are comparatively minor, and are below 0.2 Ryd. However, for the higher excited levels the discrepancies are much larger, up to $\sim$1.5 Ryd, or equivalently over $1.6 \times 10^5$ cm$^{-1}$ – see for example, levels 111–127 of Ga XXII in table 3, and in a majority of cases the results of Singh and Aggarwal are lower. We discuss below the (possible) reason for these discrepancies.

In calculations with FAC it is much easier to include a larger number of configurations and their levels, or the CSFs (configuration state functions). For this reason, in the GRASP calculations Singh and Aggarwal [1] have ignored configurations with $\ell > 3$, but have (perhaps) included in FAC. As a result of this the FAC calculations have been performed with 1112 CSFs, which include all possible values of $\ell$ for $4 \leq n \leq 7$ of the
configurations listed above. Unfortunately, the 96 levels arising from these ‘additional’ 12 configurations do not lie above the 1016 included in GRASP, or above the 127 listed by them, but intermix with those. In fact they intermix quite early, from about level 100 onward. In listing the FAC energies, Singh and Aggarwal have ignored this reality and have (perhaps) listed the lowest 127 energies, and hence the discrepancies. It may be worth noting here that their calculations with both the GRASP and FAC codes had similar discrepancies in the past, for a range of ions, see for example the energy levels of five Br-like ions [2] with $38 \leq Z \leq 42$ and F-like W LXVI [3],[4].

Apart from these major discrepancies noted above, there are a few more (minor) anomalies in the tabulations provided by Singh and Aggarwal [1]. We highlight only three, i.e. (i) in table 1 the NIST energy for level 25 should be 79.466 Ryd, and not 7.9E+07, (ii) the level 88 in table 1 should be $^3P_0^0$, and not $^3P_0^r$, and finally (iii) the level 48 in table 2 should be $^3P_0^r$, and not $^3P_0^r$, as listed. Similarly, for a few levels the FAC1 energies listed by them are non degenerate, but is not the case in our FAC2 calculations, see for example the levels 74/75 in their table 1 for Cu XX, and 62/63, 88/89, 102/103 and 106/107 in table 3 for Ga XXII. There are a few more anomalies in other tables as well, but we will like to particularly comment on the comparisons of energies shown in their table 4, because the discrepancies for a few levels appear to be very significant (~2 Ryd) – see for example, levels 3 and 5, i.e. $2s^22p^53s^1P_1$ and $2s^22p^53s^3P_1$. This is because these levels (and many more) are highly mixed and their ordering may change with the change in CI. For this reason such levels are not given an LSJ$^\pi$ designations in the NIST listings, but only their $J$ values.

3 Radiative rates

Singh and Aggarwal [1] have also listed A-values for some resonance transitions in tables 5–7, but for four types, i.e. electric and magnetic dipole (E1 and M1) and quadrupole (E2 and M2). In table 9 they have compared their results with the earlier ones of Hibbert et al [5] for a few E1 transitions, and have ‘concluded’ a good agreement, whereas we find that the listed A-values of [5] are larger by a factor of three, for all transitions and ions. This is not only contrary to their conclusion but also inconsistent with their subsequent results of $\tau$ (listed and compared in table 10) for which there are no discrepancies. A closer look at the tables of Hibbert et al [5] reveals that they have listed weighted A-values, i.e. $\omega A$, and for the transitions in table 9 of Singh and Aggarwal, the statistical weight $\omega$ is exactly three, and hence the discrepancies. Similar discrepancies, and for the same reason, were also noted earlier [6] with their results for the transitions of Sr XXX.

4 Conclusions

In this paper we have highlighted some of the errors and discrepancies in the reported data of Singh and Aggarwal [1] for 127 levels of three Ne-like ions: Cu XX, Zn XXI and Ga XXII. Particularly for energy levels, their listed results with the FAC calculations are incorrect, by up to 1.5 Ryd. Apart from this, their listed 127 levels of the $2s^22p^6$, $2s^22p^53\ell$, $2s^22p^63\ell$, $2s^22p^54\ell$, $2s2p^64\ell$ and $2s2p^55\ell$ ($\ell \leq 3$) configurations are not the lowest in energy, because some from the neglected configurations, such as $2s2p^55g$, intermix. Therefore, there is scope for the improvement over their work. For the similar reason, some of the listed lifetimes may be affected because some of the missing transitions may make a contribution. Furthermore, the limited data reported in their paper for the A-values are not of much use, because for any modelling or diagnostic application a complete set of data covering all transitions is preferred.

With the ready availability of various atomic structure codes it has become comparatively easy to produce atomic data. However, it is still not straightforward to produce accurate and reliable data which can be applied with confidence. Most of the discrepancies, often noted in various atomic parameters, including energy levels and radiative rates, are because of the non practical assumptions made or inadequate comparisons and
assessments. Many times the assessment of accuracy is based on speculations rather than a rigorous and robust analysis. Several instances of large discrepancies in various parameters, and their possible simple resolutions, have recently been highlighted by us [7].

A complete set of data for energy levels, A-values and lifetimes for all three ions (Cu XX, Zn XXI and Ga XXII) are reported in our recent paper [8] and can be confidently applied in the modelling of plasmas.

References

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| Index | Configuration | Level | GRASP | FAC1 | FAC2 |
|-------|---------------|-------|-------|------|------|
| 1     | 2s$^2$2p$^5$ | $^1$S$_0$ | 0.0000 | 0.0000 | 0.0000 |
| 2     | 2s$^2$2p$^5$3s | $^3$P$_2$ | 70.6919 | 70.7705 | 70.63754 |
| 3     | 2s$^2$2p$^5$3s | $^1$P$_1$ | 70.8653 | 70.9535 | 70.80313 |
| 4     | 2s$^2$2p$^5$3s | $^3$P$_0$ | 72.2166 | 72.2977 | 72.15617 |
| 5     | 2s$^2$2p$^5$3s | $^1$P$_1$ | 72.3172 | 72.4053 | 72.25147 |
| 6     | 2s$^2$2p$^5$3p | $^3$S$_1$ | 73.3742 | 73.4435 | 73.32529 |
| 7     | 2s$^2$2p$^5$3p | $^3$D$_2$ | 73.6392 | 73.7184 | 73.58100 |
| 8     | 2s$^2$2p$^5$3p | $^3$D$_4$ | 73.8841 | 73.9592 | 73.83012 |
| 9     | 2s$^2$2p$^5$3p | $^1$P$_1$ | 73.9583 | 74.0387 | 73.90212 |
| 10    | 2s$^2$2p$^5$3p | $^3$P$_2$ | 74.1445 | 74.2258 | 74.08412 |
| 11    | 2s$^2$2p$^5$3p | $^3$P$_0$ | 74.7588 | 74.8408 | 74.68418 |
| 12    | 2s$^2$2p$^5$3p | $^3$D$_1$ | 75.1061 | 75.1872 | 75.04516 |
| 13    | 2s$^2$2p$^5$3p | $^3$P$_1$ | 75.4856 | 75.5648 | 75.42378 |
| 14    | 2s$^2$2p$^5$3p | $^1$D$_2$ | 75.5343 | 75.6162 | 75.46973 |
| 15    | 2s$^2$2p$^5$3p | $^1$S$_0$ | 76.6747 | 76.7670 | 76.49453 |
| 16    | 2s$^2$2p$^5$3d | $^3$P$_0$ | 77.3901 | 77.4741 | 77.30283 |
| 17    | 2s$^2$2p$^5$3d | $^3$P$_2$ | 77.4886 | 77.5468 | 77.40108 |
| 18    | 2s$^2$2p$^5$3d | $^3$P$_0$ | 77.6721 | 77.7263 | 77.58429 |
| 19    | 2s$^2$2p$^5$3d | $^3$F$_4$ | 77.6720 | 77.7326 | 77.58456 |
| 20    | 2s$^2$2p$^5$3d | $^3$F$_3$ | 77.7222 | 77.7778 | 77.62885 |
| 21    | 2s$^2$2p$^5$3d | $^1$D$_2$ | 77.8832 | 77.9411 | 77.78970 |
| 22    | 2s$^2$2p$^5$3d | $^3$D$_3$ | 77.9900 | 78.0527 | 77.89623 |
| 23    | 2s$^2$2p$^5$3d | $^3$D$_1$ | 78.4870 | 78.5407 | 78.37643 |
| 24    | 2s$^2$2p$^5$3d | $^3$F$_2$ | 79.2339 | 79.2971 | 79.14201 |
| 25    | 2s$^2$2p$^5$3d | $^3$D$_2$ | 79.3136 | 79.3733 | 79.21323 |
| 26    | 2s$^2$2p$^5$3d | $^1$F$_3$ | 79.3771 | 79.5361 | 79.27460 |
| 27    | 2s$^2$2p$^5$3d | $^1$P$_1$ | 79.9972 | 80.0433 | 79.85892 |
| 28    | 2s$^2$p$^3$s | $^3$S$_1$ | 82.6714 | 82.7901 | 82.65656 |
| 29    | 2s$^2$p$^3$s | $^1$S$_0$ | 83.2709 | 83.3917 | 83.24921 |
| 30    | 2s$^2$p$^6$3p | $^3$P$_0$ | 85.5424 | 85.6516 | 85.54147 |
| 31    | 2s$^2$p$^6$3p | $^3$P$_2$ | 85.5878 | 85.6984 | 85.58796 |
| 32    | 2s$^2$p$^6$3p | $^3$P$_0$ | 85.8917 | 86.0002 | 85.89172 |
| 33    | 2s$^2$p$^6$3p | $^1$P$_1$ | 86.0536 | 86.1689 | 86.05657 |
| 34    | 2s$^2$p$^6$3d | $^3$D$_1$ | 89.5212 | 89.5967 | 89.48917 |
| 35    | 2s$^2$p$^6$3d | $^3$D$_2$ | 89.5402 | 89.6158 | 89.50820 |
| 36    | 2s$^2$p$^6$3d | $^3$D$_3$ | 89.5777 | 89.6530 | 89.54538 |
| 37    | 2s$^2$p$^6$3d | $^1$D$_2$ | 90.0109 | 90.1029 | 89.97868 |
| 38    | 2s$^2$p$^6$4s | $^3$P$_2$ | 95.5294 | 95.5800 | 95.60201 |
| 39    | 2s$^2$p$^6$4s | $^1$P$_1$ | 95.5845 | 95.6373 | 95.65949 |
| 40    | 2s$^2$p$^6$4p | $^3$S$_1$ | 96.6490 | 96.6972 | 96.71725 |
| 41    | 2s$^2$p$^6$4p | $^3$D$_2$ | 96.7127 | 96.7619 | 96.78351 |
| 42    | 2s$^2$p$^6$4p | $^3$D$_3$ | 96.8157 | 96.8639 | 96.88505 |
| 43    | 2s$^2$p$^6$4p | $^1$P$_1$ | 96.8430 | 96.8919 | 96.91355 |
| 44    | 2s$^2$p$^6$4p | $^3$P$_2$ | 96.9026 | 96.9524 | 96.97429 |
| 45    | 2s$^2$p$^6$4s | $^3$P$_0$ | 97.0570 | 97.1121 | 97.13254 |
| Index | Configuration | Level | GRASP  | FAC1   | FAC2   |
|-------|---------------|-------|--------|--------|--------|
| 46    | 2s² 2p⁵ 4s    | 3P⁰  | 97.0837| 97.1400| 97.16054|
| 47    | 2s² 2p⁵ 4p    | 3P⁰  | 97.2722| 97.3121| 97.33091|
| 48    | 2s² 2p⁵ 4d    | 3P⁰  | 98.1282| 98.1747| 98.19264|
| 49    | 2s² 2p⁵ 4d    | 3P⁰  | 98.1698| 98.2154| 98.23391|
| 50    | 2s² 2p⁵ 4d    | 3P⁰  | 98.2236| 98.2687| 98.28776|
| 51    | 2s² 2p⁵ 4d    | 3P⁰  | 98.2391| 98.2691| 98.30323|
| 52    | 2s² 2p⁵ 4d    | 3P⁰  | 98.2405| 98.2832| 98.30276|
| 53    | 2s² 2p⁵ 4p    | 3P⁰  | 98.2169| 98.2833| 98.28912|
| 54    | 2s² 2p⁵ 4d    | 1D²  | 98.2988| 98.3402| 98.36112|
| 55    | 2s² 2p⁵ 4d    | 3D⁰  | 98.3389| 98.3796| 98.40092|
| 56    | 2s² 2p⁵ 4p    | 3P⁰  | 98.3627| 98.4162| 98.43573|
| 57    | 2s² 2p⁵ 4p    | 1D²  | 98.3833| 98.4372| 98.45709|
| 58    | 2s² 2p⁵ 4d    | 1P⁰  | 98.5765| 98.6104| 98.63273|
| 59    | 2s² 2p⁵ 4p    | 1S⁰  | 98.5960| 98.6370| 98.65317|
| 60    | 2s² 2p⁵ 4f    | 3D¹  | 98.9161| 98.9769| 98.99990|
| 61    | 2s² 2p⁵ 4f    | 1G⁴  | 98.9238| 98.9864| 99.00787|
| 62    | 2s² 2p⁵ 4f    | 3D²  | 98.9295| 98.9910| 99.01653|
| 63    | 2s² 2p⁵ 4f    | 3G⁵  | 98.9316| 98.9943| 99.01272|
| 64    | 2s² 2p⁵ 4f    | 3F⁴  | 98.9661| 99.0296| 99.05234|
| 65    | 2s² 2p⁵ 4f    | 1D²  | 98.9687| 99.0363| 99.05705|
| 66    | 2s² 2p⁵ 4f    | 1F³  | 98.9754| 99.0399| 99.06224|
| 67    | 2s² 2p⁵ 4f    | 3F⁴  | 98.9852| 99.0500| 99.07230|
| 68    | 2s² 2p⁵ 4d    | 3F⁵  | 99.7552| 99.8037| 99.82186|
| 69    | 2s² 2p⁵ 4d    | 3D³  | 99.7861| 99.8341| 99.85231|
| 70    | 2s² 2p⁵ 4d    | 1F³  | 99.8147| 99.8615| 99.88031|
| 71    | 2s² 2p⁵ 4d    | 3D⁰  | 99.9821| 100.0200| 100.04225|
| 72    | 2s² 2p⁵ 4f    | 3G³  | 100.4694| 100.5370| 100.55752|
| 73    | 2s² 2p⁵ 4f    | 3G⁴  | 100.4834| 100.5510| 100.57141|
| 74    | 2s² 2p⁵ 4f    | 3F²  | 100.4875| 100.5580| 100.57841|
| 75    | 2s² 2p⁵ 4f    | 3D³  | 100.4906| 100.5580| 100.57952|
| 76    | 2s² 2p⁵ 5s    | 3P⁴  | 106.2758| 106.3310| 106.35044|
| 77    | 2s² 2p⁵ 5s    | 1P⁴  | 106.3043| 106.3590| 106.37932|
| 78    | 2s² 2p⁵ 5p    | 3S¹  | 106.8108| 106.8650| 106.88153|
| 79    | 2s² 2p⁵ 5p    | 3D²  | 106.8680| 106.9210| 106.94092|
| 80    | 2s² 2p⁵ 5p    | 3D³  | 106.9194| 106.9730| 106.99187|
| 81    | 2s² 2p⁵ 5p    | 1P¹  | 106.9290| 106.9820| 107.00132|
| 82    | 2s² 2p⁵ 5p    | 3P²  | 106.9625| 107.0150| 107.03518|
| 83    | 2s² 2p⁵ 5p    | 1S⁰  | 107.1485| 107.1940| 107.21065|
| 84    | 2s² 2p⁵ 5p    | 3S¹  | 107.4520| 107.4750| 107.49048|
| 85    | 2s² 2p⁵ 5d    | 3P⁰  | 107.5565| 107.6170| 107.63197|
| 86    | 2s² 2p⁵ 5d    | 3P⁰  | 107.5785| 107.6370| 107.65339|
| 87    | 2s² 2p⁵ 5d    | 3F⁴  | 107.6066| 107.6480| 107.68114|
| 88    | 2s² 2p⁵ 5d    | 3F⁴  | 107.6141| 107.6640| 107.68710|
| 89    | 2s² 2p⁵ 5d    | 3P²  | 107.6138| 107.6690| 107.68814|
| 90    | 2s² 2p⁵ 5d    | 1D²  | 107.6414| 107.6710| 107.71408|
| Index | Configuration | Level  | GRASP  | FAC1  | FAC2  |
|------|---------------|--------|--------|-------|-------|
| 91   | 2s2p^64s      | ^1S_0  | 107.6356 | 107.6950 | 107.66429 |
| 92   | 2s^22p^5d     | ^3D_3  | 107.6611 | 107.7140 | 107.73308 |
| 93   | 2s^22p^5d     | ^1P_y | 107.7641 | 107.8130 | 107.83283 |
| 94   | 2s^22p^5s     | ^3P_0  | 107.7971 | 107.8560 | 107.87410 |
| 95   | 2s^22p^5s     | ^3P_y | 107.8348 | 107.8900 | 107.90797 |
| 96   | 2s^22p^5f     | ^3D_1  | 107.9400 | 108.0060 | 108.02713 |
| 97   | 2s^22p^5f     | ^3D_2  | 107.9508 | 108.0180 | 108.03856 |
| 98   | 2s^22p^5f     | ^3G_4  | 107.9545 | 108.0220 | 108.04248 |
| 99   | 2s^22p^5f     | ^3G_5  | 107.9565 | 108.0240 | 108.04405 |
| 100  | 2s^22p^5f     | ^3D_3  | 107.9710 | 108.0390 | 108.05925 |
| 101  | 2s^22p^5f     | ^1D_2  | 107.9778 | 108.0400 | 108.06748 |
| 102  | 2s^22p^5f     | ^1F_3  | 107.9792 | 108.0440 | 108.06792 |
| 103  | 2s^22p^5f     | ^3F_4  | 107.9848 | 108.0470 | 108.07363 |
| 104  | 2s^22p^5f     | ^3D_4  | 108.3864 | 108.0480 | 108.46130 |
| 105  | 2s^22p^5f     | ^3P_1  | 108.4674 | 108.0530 | 108.54401 |
| 106  | 2s^22p^5f     | ^1D_2  | 108.4687 | 108.0550 | 108.54325 |
| 107  | 2s^22p^5f     | ^3P_0  | 108.5485 | 108.0580 | 108.61346 |
| 108  | 2s^2p^64p     | ^3P_y | 108.6111 | 108.0610 | 108.64568 |
| 109  | 2s^2p^64p     | ^3P_y | 108.6158 | 108.0630 | 108.65070 |
| 110  | 2s^2p^64p     | ^3P_y | 108.7342 | 108.0690 | 108.76862 |
| 111  | 2s^2p^64p     | ^1P_y | 108.7914 | 108.0720 | 108.82734 |
| 112  | 2s^22p^5d     | ^3F_2  | 109.1362 | 108.4430 | 109.21307 |
| 113  | 2s^22p^5d     | ^3D_2  | 109.1553 | 108.5250 | 109.23176 |
| 114  | 2s^22p^5d     | ^1F_3  | 109.1658 | 108.5260 | 109.24195 |
| 115  | 2s^22p^5d     | ^3D_3  | 109.2410 | 108.6000 | 109.31123 |
| 116  | 2s^22p^5f     | ^3G_3  | 109.4909 | 108.6300 | 109.58144 |
| 117  | 2s^22p^5f     | ^3F_3  | 109.4927 | 108.6350 | 109.58350 |
| 118  | 2s^22p^5f     | ^3F_2  | 109.4972 | 108.7540 | 109.58903 |
| 119  | 2s^22p^5f     | ^3G_4  | 109.4997 | 108.8100 | 109.59068 |
| 120  | 2s^2p^64d     | ^3D_1  | 110.1045 | 109.1970 | 110.12934 |
| 121  | 2s^2p^64d     | ^3D_2  | 110.1152 | 109.2160 | 110.14050 |
| 122  | 2s^2p^64d     | ^3D_3  | 110.1349 | 109.2250 | 110.16087 |
| 123  | 2s^2p^64d     | ^1D_2  | 110.2809 | 109.2940 | 110.30125 |
| 124  | 2s^2p^64f     | ^3F_2  | 110.7921 | 109.5630 | 110.84024 |
| 125  | 2s^2p^64f     | ^3F_3  | 110.7941 | 109.5650 | 110.84754 |
| 126  | 2s^2p^64f     | ^3F_4  | 110.8017 | 109.5710 | 110.85810 |
| 127  | 2s^2p^64f     | ^1F_3  | 110.8157 | 109.5720 | 110.86835 |

GRASP: Earlier results of Singh and Aggarwal [1] with the GRASP code

FAC1: Earlier results of Singh and Aggarwal [1] with the FAC code

FAC2: Present results with the FAC code
| Index | Configuration | Level | GRASP | FAC1 | FAC2 |
|-------|---------------|-------|-------|------|------|
| 1     | $2s^22p^5$    | $^1S_0$ | 0.0000 | 0.0000 | 0.0000 |
| 2     | $2s^22p^53s$  | $^3P_2^0$ | 77.0829 | 77.1622 | 77.02974 |
| 3     | $2s^22p^53s$  | $^1P_1^0$ | 77.2657 | 77.3546 | 77.20457 |
| 4     | $2s^22p^53s$  | $^3P_0^0$ | 78.8614 | 78.9435 | 78.80181 |
| 5     | $2s^22p^53s$  | $^3P_1^0$ | 78.9649 | 79.0539 | 78.90022 |
| 6     | $2s^22p^53p$  | $^3S_1$ | 79.9196 | 79.9897 | 79.87126 |
| 7     | $2s^22p^53p$  | $^3D_2$ | 80.1804 | 80.2601 | 80.12322 |
| 8     | $2s^22p^53p$  | $^3D_4$ | 80.4828 | 80.5583 | 80.42992 |
| 9     | $2s^22p^53p$  | $^1P_1$ | 80.5515 | 80.6322 | 80.49657 |
| 10    | $2s^22p^53p$  | $^3P_2$ | 80.7564 | 80.8381 | 80.69710 |
| 11    | $2s^22p^53p$  | $^3P_0$ | 81.4461 | 81.5289 | 81.37004 |
| 12    | $2s^22p^53p$  | $^3D_1$ | 81.8956 | 81.9773 | 81.83533 |
| 13    | $2s^22p^53p$  | $^3P_1$ | 82.3366 | 82.4164 | 82.27576 |
| 14    | $2s^22p^53p$  | $^1D_2$ | 82.3920 | 82.4746 | 82.32825 |
| 15    | $2s^22p^53p$  | $^1S_0$ | 83.4967 | 83.5888 | 83.32059 |
| 16    | $2s^22p^53d$  | $^3P_0^0$ | 84.1579 | 84.2146 | 84.07169 |
| 17    | $2s^22p^53d$  | $^3P_1^0$ | 84.2661 | 84.3240 | 84.17962 |
| 18    | $2s^22p^53d$  | $^3P_2^0$ | 84.4671 | 84.5172 | 84.38020 |
| 19    | $2s^22p^53d$  | $^3F_4^0$ | 84.4631 | 84.5274 | 84.37681 |
| 20    | $2s^22p^53d$  | $^3F_3^0$ | 84.5079 | 84.5635 | 84.41571 |
| 21    | $2s^22p^53d$  | $^1D_2$ | 84.6811 | 84.7391 | 84.58873 |
| 22    | $2s^22p^53d$  | $^3D_3$ | 84.8000 | 84.8624 | 84.70740 |
| 23    | $2s^22p^53d$  | $^3D_5^0$ | 85.3457 | 85.3986 | 85.23471 |
| 24    | $2s^22p^53d$  | $^3F_2^0$ | 86.2698 | 86.3332 | 86.17882 |
| 25    | $2s^22p^53d$  | $^3D_2^0$ | 86.3610 | 86.4209 | 86.26147 |
| 26    | $2s^22p^53d$  | $^1F_3^0$ | 86.4317 | 86.4909 | 86.32999 |
| 27    | $2s^22p^53d$  | $^1P_1^0$ | 87.0583 | 87.1054 | 86.92262 |
| 28    | $2s^2p^63s$   | $^3S_1$ | 89.7723 | 89.8922 | 89.75857 |
| 29    | $2s^2p^63s$   | $^1S_0$ | 90.4013 | 90.5230 | 90.38050 |
| 30    | $2s^2p^63p$   | $^3P_0^0$ | 92.7900 | 92.9003 | 92.78983 |
| 31    | $2s^2p^63p$   | $^3P_1^0$ | 92.8395 | 92.9512 | 92.84050 |
| 32    | $2s^2p^63p$   | $^3P_2^0$ | 93.2025 | 93.3119 | 93.20325 |
| 33    | $2s^2p^63p$   | $^1P_1^0$ | 93.3696 | 93.4859 | 93.37355 |
| 34    | $2s^2p^63d$   | $^3D_1$ | 97.0103 | 97.0861 | 96.97910 |
| 35    | $2s^2p^63d$   | $^3D_2$ | 97.0332 | 97.1092 | 97.00204 |
| 36    | $2s^2p^63d$   | $^3D_3$ | 97.0790 | 97.1547 | 97.04758 |
| 37    | $2s^2p^63d$   | $^1D_2$ | 97.5360 | 97.6286 | 97.50471 |
| 38    | $2s^2p^64s$   | $^3P_0^0$ | 104.2275 | 104.2790 | 104.30032 |
| 39    | $2s^2p^64s$   | $^1P_1^0$ | 104.2857 | 104.3390 | 104.36092 |
| 40    | $2s^2p^64p$   | $^3S_1$ | 105.4109 | 105.4600 | 105.47927 |
| 41    | $2s^2p^64p$   | $^3D_2$ | 105.4742 | 105.5240 | 105.54500 |
| 42    | $2s^2p^64p$   | $^3D_3$ | 105.6007 | 105.6500 | 105.67009 |
| 43    | $2s^2p^64p$   | $^1P_1$ | 105.6269 | 105.6760 | 105.69740 |
| 44    | $2s^2p^64p$   | $^3P_2$ | 105.6926 | 105.7430 | 105.76432 |
| 45    | $2s^2p^64s$   | $^3P_0^0$ | 106.0096 | 106.0660 | 106.08551 |
| Index | Configuration | Level  | GRASP | FAC1  | FAC2  |
|-------|---------------|--------|-------|-------|-------|
| 46    | 2s²2p³4p      | ³P₀   | 106.0372 | 106.0950 | 106.14487 |
| 47    | 2s²2p⁵4s      | ³P₁   | 106.0873 | 106.1270 | 106.11443 |
| 48    | 2s²2p⁵4d      | ³P₀   | 106.9794 | 107.0270 | 107.04406 |
| 49    | 2s²2p⁵4d      | ³P₁   | 107.0244 | 107.0710 | 107.08862 |
| 50    | 2s²2p⁵4d      | ³F₁   | 107.0839 | 107.1300 | 107.14819 |
| 51    | 2s²2p⁵4d      | ³F₂   | 107.0977 | 107.1410 | 107.16050 |
| 52    | 2s²2p⁵4d      | ³P₂   | 107.0998 | 107.1450 | 107.16348 |
| 53    | 2s²2p⁵4d      | ¹D₂   | 107.1607 | 107.2030 | 107.22317 |
| 54    | 2s²2p⁵4d      | ³D₃   | 107.2059 | 107.2470 | 107.26792 |
| 55    | 2s²2p⁵4p      | ³D₁   | 107.2311 | 107.2840 | 107.30363 |
| 56    | 2s²2p⁵4d      | ¹P₀   | 107.4028 | 107.4570 | 107.47601 |
| 57    | 2s²2p⁵4p      | ³P₁   | 107.4247 | 107.4800 | 107.51529 |
| 58    | 2s²2p⁵4p      | ¹D₂   | 107.4593 | 107.4940 | 107.49883 |
| 59    | 2s²2p⁵4p      | ¹S₀   | 107.6192 | 107.6620 | 107.67708 |
| 60    | 2s²2p⁵4f      | ³D₁   | 107.8197 | 107.8810 | 107.90350 |
| 61    | 2s²2p⁵4f      | ¹G₄   | 107.8297 | 107.8930 | 107.91365 |
| 62    | 2s²2p⁵4f      | ³D₂   | 107.8378 | 107.8990 | 107.92260 |
| 63    | 2s²2p⁵4f      | ³G₅   | 107.8372 | 107.9010 | 107.92036 |
| 64    | 2s²2p⁵4f      | ³F₃   | 107.8752 | 107.9390 | 107.96143 |
| 65    | 2s²2p⁵4f      | ¹D₂   | 107.8781 | 107.9470 | 107.96655 |
| 66    | 2s²2p⁵4f      | ¹F₃   | 107.8853 | 107.9510 | 107.97209 |
| 67    | 2s²2p⁵4f      | ³F₄   | 107.8969 | 107.9620 | 107.98395 |
| 68    | 2s²2p⁵4d      | ³F₂   | 108.8657 | 108.9160 | 108.93279 |
| 69    | 2s²2p⁵4d      | ³D₂   | 108.9023 | 108.9520 | 108.96901 |
| 70    | 2s²2p⁵4d      | ¹F₃   | 108.9329 | 108.9810 | 108.99892 |
| 71    | 2s²2p⁵4d      | ³D₁   | 109.1018 | 109.1430 | 109.16225 |
| 72    | 2s²2p⁵4f      | ³G₃   | 109.6309 | 109.7000 | 109.71927 |
| 73    | 2s²2p⁵4f      | ³G₄   | 109.6476 | 109.7170 | 109.73579 |
| 74    | 2s²2p⁵4f      | ³F₂   | 109.6499 | 109.7220 | 109.74110 |
| 75    | 2s²2p⁵4f      | ³D₃   | 109.6543 | 109.7230 | 109.74351 |
| 76    | 2s²2p⁵5s      | ³P₂   | 116.0031 | 116.0590 | 116.07773 |
| 77    | 2s²2p⁵5s      | ¹P₀   | 116.0333 | 116.0900 | 116.10839 |
| 78    | 2s²2p⁵5p      | ³S₁   | 116.5293 | 116.5800 | 116.59354 |
| 79    | 2s²2p⁵5p      | ³D₂   | 116.6284 | 116.6820 | 116.70123 |
| 80    | 2s²2p⁵5p      | ¹P₁   | 116.6920 | 116.7450 | 116.76329 |
| 81    | 2s²2p⁵5p      | ³D₃   | 116.6915 | 116.7460 | 116.76395 |
| 82    | 2s²2p⁵5p      | ³P₂   | 116.7372 | 116.7910 | 116.80986 |
| 83    | 2s²2p⁵5p      | ¹S₀   | 116.9031 | 116.9370 | 116.96329 |
| 84    | 2s²p⁶4s       | ³S₁   | 116.9081 | 116.9460 | 116.95404 |
| 85    | 2s²p⁶4s       | ¹S₀   | 117.0788 | 117.0960 | 117.10867 |
| 86    | 2s²2p⁵5d      | ³P₀   | 117.3596 | 117.4210 | 117.43507 |
| 87    | 2s²2p⁵5d      | ³P₁   | 117.3839 | 117.4440 | 117.45881 |
| 88    | 2s²2p⁵5d      | ³F₁   | 117.4162 | 117.4750 | 117.49099 |
| 89    | 2s²2p⁵5d      | ³F₂   | 117.4217 | 117.4780 | 117.49515 |
| 90    | 2s²2p⁵5d      | ³P₂   | 117.4232 | 117.4810 | 117.49727 |
| Index | Configuration | Level  | GRASP     | FAC1     | FAC2     |
|-------|---------------|--------|-----------|----------|----------|
| 91    | $2s^22p^5d$   | $^1D_2^0$ | 117.4517  | 117.5070 | 117.52450 |
| 92    | $2s^22p^5d$   | $^3D_3^0$ | 117.4739  | 117.5280 | 117.54601 |
| 93    | $2s^22p^5d$   | $^1P_1^0$ | 117.5966  | 117.6430 | 117.66148 |
| 94    | $2s^22p^5f$   | $^3D_1^0$ | 117.7695  | 117.8100 | 117.85645 |
| 95    | $2s^22p^5f$   | $^3D_2^0$ | 117.7819  | 117.8370 | 117.86942 |
| 96    | $2s^22p^5f$   | $^3G_4^0$ | 117.7517  | 117.8470 | 117.87419 |
| 97    | $2s^22p^5f$   | $^3G_5^0$ | 117.7864  | 117.8500 | 117.87666 |
| 98    | $2s^22p^5s$   | $^3P_0^0$ | 117.7893  | 117.8550 | 117.82523 |
| 99    | $2s^22p^5f$   | $^3D_3^0$ | 117.8040  | 117.8580 | 117.89209 |
| 100   | $2s^22p^5f$   | $^1D_2^0$ | 117.8117  | 117.8720 | 117.90127 |
| 101   | $2s^22p^5f$   | $^1F_3^0$ | 117.8129  | 117.8760 | 117.90144 |
| 102   | $2s^22p^5f$   | $^3F_4^0$ | 117.8195  | 117.8800 | 117.90820 |
| 103   | $2s^22p^5s$   | $^3P_1^0$ | 117.7886  | 117.8820 | 117.86364 |
| 104   | $2s^22p^4p$   | $^3P_1^0$ | 118.0939  | 117.8830 | 118.13043 |
| 105   | $2s^22p^4p$   | $^3P_0^0$ | 118.1060  | 117.8890 | 118.14479 |
| 106   | $2s^22p^4p$   | $^3P_2^0$ | 118.2282  | 117.8920 | 118.26240 |
| 107   | $2s^22p^4p$   | $^1P_1^0$ | 118.2918  | 117.8960 | 118.32829 |
| 108   | $2s^22p^5p$   | $^3D_3^0$ | 118.3992  | 117.8980 | 118.47430 |
| 109   | $2s^22p^5p$   | $^3P_1^0$ | 118.4932  | 117.9010 | 118.56895 |
| 110   | $2s^22p^5p$   | $^1D_2^0$ | 118.4940  | 117.9080 | 118.57005 |
| 111   | $2s^22p^5p$   | $^3P_0^0$ | 118.5667  | 117.9110 | 118.63262 |
| 112   | $2s^22p^5d$   | $^3F_2^0$ | 119.1983  | 118.1150 | 119.27555 |
| 113   | $2s^22p^5d$   | $^3D_2^0$ | 119.2183  | 118.1290 | 119.29566 |
| 114   | $2s^22p^5d$   | $^1F_3^0$ | 119.2316  | 118.2480 | 119.30828 |
| 115   | $2s^22p^5d$   | $^3D_1^0$ | 119.3062  | 118.3120 | 119.37708 |
| 116   | $2s^22p^5f$   | $^3F_3^0$ | 119.5431  | 118.4580 | 119.61725 |
| 117   | $2s^22p^5f$   | $^3F_2^0$ | 119.5597  | 118.5520 | 119.63652 |
| 118   | $2s^22p^5f$   | $^3G_3^0$ | 119.5790  | 118.5530 | 119.67037 |
| 119   | $2s^22p^5f$   | $^3G_4^0$ | 119.5881  | 118.6200 | 119.67924 |
| 120   | $2s^2p^4d$    | $^3D_1^0$ | 119.6672  | 119.2610 | 119.69228 |
| 121   | $2s^2p^4f$    | $^3D_2^0$ | 119.7023  | 119.2810 | 119.74253 |
| 122   | $2s^2p^4d$    | $^3D_3^0$ | 119.7378  | 119.2930 | 119.78004 |
| 123   | $2s^2p^4d$    | $^1D_2^0$ | 119.8555  | 119.3620 | 119.87640 |
| 124   | $2s^2p^4f$    | $^3F_2^0$ | 120.3999  | 119.6030 | 120.45145 |
| 125   | $2s^2p^4f$    | $^3F_3^0$ | 120.4023  | 119.6220 | 120.46340 |
| 126   | $2s^2p^4f$    | $^3F_4^0$ | 120.4117  | 119.6530 | 120.47974 |
| 127   | $2s^2p^6f$    | $^1F_3^0$ | 120.4269  | 119.6620 | 120.48666 |

GRASP: Earlier results of Singh and Aggarwal [1] with the GRASP code
FAC1: Earlier results of Singh and Aggarwal [1] with the FAC code
FAC2: Present results with the FAC code
Table 3: Comparison of energies (in Ryd) for 127 levels of Ga XXII.

| Index | Configuration | Level | GRASP | FAC1 | FAC2 |
|-------|---------------|-------|-------|------|------|
| 1     | 2s²2p⁵       | ¹S₀   | 0.0000| 0.0000| 0.00000 |
| 2     | 2s²2p⁵3s     | ⁴P₂   | 83.7426| 83.8227| 83.69079 |
| 3     | 2s²2p⁵3s     | ¹P₁   | 83.9348| 84.0246| 83.87482 |
| 4     | 2s²2p⁵3s     | ⁴P₀   | 85.8058| 85.8890| 85.74715 |
| 5     | 2s²2p⁵3s     | ¹P₁   | 85.9122| 86.0023| 85.84867 |
| 6     | 2s²2p⁵3p     | ³S₁   | 86.7349| 86.8059| 86.68729 |
| 7     | 2s²2p⁵3p     | ³D₂   | 86.9911| 87.0714| 86.93499 |
| 8     | 2s²2p⁵3p     | ³D₄   | 87.3592| 87.4354| 87.30757 |
| 9     | 2s²2p⁵3p     | ¹P₁   | 87.4221| 87.5033| 87.36857 |
| 10    | 2s²2p⁵3p     | ³P₂   | 87.6461| 87.7284| 87.58796 |
| 11    | 2s²2p⁵3p     | ³P₀   | 88.4146| 88.4982| 88.33686 |
| 12    | 2s²2p⁵3p     | ³D₁   | 88.9853| 89.0679| 88.92588 |
| 13    | 2s²2p⁵3p     | ³P₁   | 89.4964| 89.5769| 89.43643 |
| 14    | 2s²2p⁵3p     | ¹D₂   | 89.5583| 89.6419| 89.49547 |
| 15    | 2s²2p⁵3p     | ¹S₀   | 90.6161| 90.7082| 90.44428 |
| 16    | 2s²2p⁵3d     | ³P₀   | 91.2036| 91.2602| 91.11856 |
| 17    | 2s²2p⁵3d     | ³P₁   | 91.3219| 91.3798| 91.23651 |
| 18    | 2s²2p⁵3d     | ³P₂   | 91.5411| 91.5879| 91.45519 |
| 19    | 2s²2p⁵3d     | ³F₄   | 91.5338| 91.6013| 91.44879 |
| 20    | 2s²2p⁵3d     | ³F₃   | 91.5713| 91.6270| 91.48034 |
| 21    | 2s²2p⁵3d     | ¹D₂   | 91.7574| 91.8157| 91.66630 |
| 22    | 2s²2p⁵3d     | ³D₄   | 91.8898| 91.9525| 91.79834 |
| 23    | 2s²2p⁵3d     | ³D₃   | 92.4846| 92.5370| 92.37331 |
| 24    | 2s²2p⁵3d     | ³F₂   | 93.6143| 93.6780| 93.52431 |
| 25    | 2s²2p⁵3d     | ³D₂   | 93.7190| 93.7793| 93.62042 |
| 26    | 2s²2p⁵3d     | ¹F₂   | 93.7968| 93.8564| 93.69603 |
| 27    | 2s²2p⁵3d     | ¹P₁   | 94.4270| 94.4753| 94.29389 |
| 28    | 2s²p⁶3s      | ³S₁   | 97.1756| 97.2969| 97.16302 |
| 29    | 2s²p⁶3s      | ¹S₀   | 97.8344| 97.9571| 97.81450 |
| 30    | 2s²p⁶3p      | ³P₀   | 100.3409| 100.4520| 100.34146 |
| 31    | 2s²p⁶3p      | ³P₁   | 100.3943| 100.5070| 100.39630 |
| 32    | 2s²p⁶3p      | ³P₂   | 100.8246| 100.9350| 100.82625 |
| 33    | 2s²p⁶3p      | ¹P₁   | 100.9970| 101.1140| 101.00202 |
| 34    | 2s²p⁶3d      | ³D₁   | 104.8107| 104.8870| 104.78048 |
| 35    | 2s²p⁶3d      | ³D₂   | 104.8380| 104.9150| 104.80786 |
| 36    | 2s²p⁶3d      | ³D₃   | 104.8936| 104.9700| 104.86314 |
| 37    | 2s²p⁶3d      | ¹D₂   | 105.3738| 105.4670| 105.34357 |
| 38    | 2s²p⁶3s      | ³P₀   | 113.2984| 113.3510| 113.37141 |
| 39    | 2s²p⁶4s      | ³P₂   | 113.3597| 113.4140| 113.43512 |
| 40    | 2s²p⁶4p      | ³S₁   | 114.5460| 114.5960| 114.61448 |
| 41    | 2s²p⁶4p      | ³D₂   | 114.6088| 114.6590| 114.67960 |
| 42    | 2s²p⁶4p      | ³D₃   | 114.7622| 114.8120| 114.83161 |
| 43    | 2s²p⁶4p      | ¹P₁   | 114.7872| 114.8380| 114.85764 |
| 44    | 2s²p⁶4p      | ³P₂   | 114.8591| 114.9100| 114.93084 |
| 45    | 2s²p⁶4p      | ³P₀   | 115.2783| 115.3180| 115.33489 |
| Index | Configuration | Level | GRASP | FAC1 | FAC2 |
|-------|---------------|-------|-------|------|------|
| 46    | $2s^22p^3s$   | $^3P_0$ | 115.3657 | 115.4230 | 115.44212 |
| 47    | $2s^22p^3s$   | $^3P_1$ | 115.3941 | 115.4530 | 115.47182 |
| 48    | $2s^22p^3d$   | $^3P_0$ | 116.2073 | 116.2560 | 116.27206 |
| 49    | $2s^22p^3d$   | $^3P_1$ | 116.2556 | 116.3030 | 116.32000 |
| 50    | $2s^22p^3d$   | $^3P_2$ | 116.3215 | 116.3680 | 116.38595 |
| 51    | $2s^22p^3d$   | $^3F_3$ | 116.3313 | 116.3760 | 116.39421 |
| 52    | $2s^22p^3d$   | $^3P_2$ | 116.3374 | 116.3830 | 116.40111 |
| 53    | $2s^22p^3d$   | $^1D_2$ | 116.3996 | 116.4430 | 116.46217 |
| 54    | $2s^22p^3d$   | $^3D_3$ | 116.4501 | 116.4920 | 116.51226 |
| 55    | $2s^22p^3p$   | $^3D_1$ | 116.6492 | 116.7040 | 116.72211 |
| 56    | $2s^22p^3d$   | $^1P_0$ | 116.7194 | 116.7540 | 116.77510 |
| 57    | $2s^22p^3p$   | $^3P_1$ | 116.8501 | 116.9060 | 116.92368 |
| 58    | $2s^22p^3p$   | $^1D_2$ | 116.8734 | 116.9300 | 116.94786 |
| 59    | $2s^22p^3p$   | $^1S_0$ | 117.0469 | 117.0910 | 117.10551 |
| 60    | $2s^22p^3f$   | $^3D_1$ | 117.1009 | 117.1630 | 117.18462 |
| 61    | $2s^22p^3f$   | $^1G_4$ | 117.1128 | 117.1770 | 117.19678 |
| 62    | $2s^22p^3f$   | $^3D_2$ | 117.1216 | 117.1860 | 117.20638 |
| 63    | $2s^22p^3f$   | $^3G_5$ | 117.1226 | 117.1860 | 117.20569 |
| 64    | $2s^22p^3f$   | $^3F_3$ | 117.1618 | 117.2270 | 117.24811 |
| 65    | $2s^22p^3f$   | $^1D_2$ | 117.1651 | 117.2350 | 117.25364 |
| 66    | $2s^22p^3f$   | $^1F_3$ | 117.1727 | 117.2390 | 117.25952 |
| 67    | $2s^22p^3f$   | $^3F_4$ | 117.1862 | 117.2530 | 117.27332 |
| 68    | $2s^22p^3d$   | $^3F_2$ | 118.3836 | 118.4350 | 118.45112 |
| 69    | $2s^22p^3d$   | $^3D_2$ | 118.4268 | 118.4780 | 118.49398 |
| 70    | $2s^22p^3d$   | $^1F_3$ | 118.4592 | 118.5090 | 118.52578 |
| 71    | $2s^22p^3d$   | $^3D_0$ | 118.6287 | 118.6710 | 118.68965 |
| 72    | $2s^22p^3f$   | $^3G_3$ | 119.2006 | 119.2710 | 119.28929 |
| 73    | $2s^22p^3f$   | $^3F_2$ | 119.2205 | 119.2910 | 119.31213 |
| 74    | $2s^22p^3f$   | $^3G_4$ | 119.2203 | 119.2940 | 119.30882 |
| 75    | $2s^22p^3f$   | $^3D_1$ | 119.2266 | 119.2970 | 119.31618 |
| 76    | $2s^22p^5s$   | $^3P_0$ | 126.1503 | 126.2080 | 126.22497 |
| 77    | $2s^22p^5s$   | $^1P_1$ | 126.1823 | 126.2400 | 126.25746 |
| 78    | $2s^2p^5s$    | $^3S_1$ | 126.5311 | 126.5660 | 126.57676 |
| 79    | $2s^2p^5p$    | $^3D_2$ | 126.8090 | 126.8570 | 126.88190 |
| 80    | $2s^2p^5p$    | $^3P_1$ | 126.8464 | 126.8640 | 126.91502 |
| 81    | $2s^2p^5s$    | $^1S_0$ | 126.8375 | 126.8970 | 126.87346 |
| 82    | $2s^2p^5p$    | $^3D_3$ | 126.8857 | 126.9410 | 126.95811 |
| 83    | $2s^2p^5p$    | $^3P_2$ | 126.9340 | 126.9870 | 127.00426 |
| 84    | $2s^2p^5p$    | $^1P_1$ | 126.9367 | 126.9890 | 127.00670 |
| 85    | $2s^2p^5p$    | $^1S_0$ | 127.1699 | 127.2120 | 127.22363 |
| 86    | $2s^2p^5d$    | $^3P_0$ | 127.5796 | 127.6410 | 127.65391 |
| 87    | $2s^2p^5d$    | $^3P_1$ | 127.6080 | 127.6690 | 127.68237 |
| 88    | $2s^2p^5d$    | $^3F_3$ | 127.6485 | 127.7090 | 127.72343 |
| 89    | $2s^2p^5d$    | $^3F_3$ | 127.6517 | 127.7090 | 127.72533 |
| 90    | $2s^2p^5d$    | $^3P_2$ | 127.6537 | 127.7130 | 127.72778 |
| Index | Configuration | Level | GRASP | FAC1 | FAC2 |
|-------|---------------|-------|-------|------|------|
| 91    | $2s^22p^5d$   | $^1D^o_2$ | 127.6843 | 127.7410 | 127.75723 |
| 92    | $2s^22p^5d$   | $^3D^o_3$ | 127.7093 | 127.7650 | 127.78153 |
| 93    | $2s^22p^5d$   | $^1P^o_1$ | 127.8377 | 127.8840 | 127.90177 |
| 94    | $2s^22p^5d$   | $^3P^o_0$ | 127.8976 | 127.9260 | 127.93940 |
| 95    | $2s^22p^5d$   | $^3P^o_1$ | 127.9415 | 127.9660 | 127.97990 |
| 96    | $2s^22p^5d$   | $^3D^o_1$ | 128.0211 | 128.0890 | 128.10779 |
| 97    | $2s^22p^5d$   | $^3D^o_2$ | 128.0352 | 128.1040 | 128.12248 |
| 98    | $2s^22p^5d$   | $^3G^o_4$ | 128.0408 | 128.1110 | 128.12852 |
| 99    | $2s^22p^5d$   | $^3G^o_5$ | 128.0448 | 128.1140 | 128.13205 |
| 100   | $2s^22p^5d$   | $^3D^o_3$ | 128.0595 | 128.1290 | 128.14743 |
| 101   | $2s^22p^5d$   | $^1D^o_2$ | 128.0683 | 128.1330 | 128.15776 |
| 102   | $2s^22p^5d$   | $^1F^o_3$ | 128.0692 | 128.1390 | 128.15764 |
| 103   | $2s^22p^5d$   | $^3F^o_4$ | 128.0770 | 128.1390 | 128.16560 |
| 104   | $2s^22p^5d$   | $^3P^o_2$ | 128.1320 | 128.1400 | 128.16658 |
| 105   | $2s^22p^5d$   | $^1P^o_1$ | 128.1372 | 128.1470 | 128.18768 |
| 106   | $2s^22p^5d$   | $^3P^o_0$ | 128.2730 | 128.1530 | 128.34535 |
| 107   | $2s^22p^5d$   | $^3P^o_1$ | 128.3123 | 128.1530 | 128.37384 |
| 108   | $2s^22p^5d$   | $^3D^o_3$ | 128.8614 | 128.1570 | 128.93661 |
| 109   | $2s^22p^5d$   | $^3P^o_1$ | 128.9718 | 128.1580 | 129.04802 |
| 110   | $2s^22p^5d$   | $^1D^o_2$ | 128.9715 | 128.1620 | 129.04755 |
| 111   | $2s^22p^5d$   | $^3P^o_0$ | 129.0372 | 128.1690 | 129.10388 |
| 112   | $2s^22p^5d$   | $^3D^o_1$ | 129.6426 | 128.1730 | 129.66847 |
| 113   | $2s^22p^5d$   | $^3D^o_2$ | 129.6433 | 128.1740 | 129.66991 |
| 114   | $2s^22p^5d$   | $^3D^o_3$ | 129.6544 | 128.3290 | 129.68199 |
| 115   | $2s^22p^5d$   | $^3F^o_2$ | 129.7133 | 128.3570 | 129.79114 |
| 116   | $2s^22p^5d$   | $^3D^o_2$ | 129.7363 | 128.9210 | 129.81430 |
| 117   | $2s^22p^5d$   | $^1F^o_3$ | 129.7509 | 129.0320 | 129.82799 |
| 118   | $2s^22p^5d$   | $^3D^o_1$ | 129.8364 | 129.0330 | 129.89680 |
| 119   | $2s^22p^5d$   | $^1D^o_2$ | 129.8254 | 129.0930 | 129.85765 |
| 120   | $2s^22p^5d$   | $^3G^o_3$ | 130.1195 | 129.6580 | 130.21107 |
| 121   | $2s^22p^5d$   | $^3G^o_4$ | 130.1302 | 129.6600 | 130.22156 |
| 122   | $2s^22p^5d$   | $^3F^o_2$ | 130.1389 | 129.6720 | 130.23026 |
| 123   | $2s^22p^5d$   | $^3F^o_3$ | 130.1457 | 129.7780 | 130.23506 |
| 124   | $2s^22p^5d$   | $^3F^o_2$ | 130.4188 | 129.8010 | 130.47401 |
| 125   | $2s^22p^5d$   | $^3F^o_3$ | 130.4215 | 129.8140 | 130.49580 |
| 126   | $2s^22p^5d$   | $^3F^o_4$ | 130.4331 | 129.8430 | 130.54657 |
| 127   | $2s^22p^5d$   | $^1F^o_3$ | 130.4497 | 129.8830 | 130.54456 |

GRASP: Earlier results of Singh and Aggarwal [1] with the GRASP code
FAC1: Earlier results of Singh and Aggarwal [1] with the FAC code
FAC2: Present results with the FAC code