Radiative rates for E1, E2, M1, and M2 transitions in F-like ions with $37 \leq Z \leq 53$

Kanti M. Aggarwal$^{a,\ast}$, Francis P. Keenan$^a$

$^a$Astrophysics Research Centre, School of Mathematics and Physics, Queen’s University Belfast, Belfast BT7 1NN, Northern Ireland, UK

Abstract
Calculations of energy levels, radiative rates and lifetimes are reported for 17 F-like ions with $37 \leq Z \leq 53$. For brevity, results are only presented among the lowest 113 levels of the $2s^22p^5$, $2s2p^6$, $2s^22p^43\ell$, $2s2p^53\ell$, and $2p^63\ell$ configurations, although the calculations have been performed for up to 501 levels in each ion. The general-purpose relativistic atomic structure package (GRASP) has been adopted for the calculations, and radiative rates (along with oscillator strengths and line strengths) are listed for all E1, E2, M1, and M2 transitions of the ions. Comparisons are made with earlier available experimental and theoretical energies, although these are limited to only a few levels for most ions. Therefore for additional accuracy assessments, particularly for energy levels, analogous calculations have been performed with the Flexible Atomic Code (FAC), for up to 72 259 levels. Limited previous results are available for radiative rates for comparison purposes, and no large discrepancy is observed for any transition and/or ion.

Received: 5 November 2015, Accepted: 30 November 2015

Keywords: F-like ions, energy levels, radiative rates, oscillator strengths, line strengths, lifetimes

$^\ast$Corresponding author.
Email address: K.Aggarwal@qub.ac.uk (Kanti M. Aggarwal)
1. Introduction

Transitions of F-like ions are prominent in high temperature plasmas [1, 2] and are useful for diagnostics. While transitions of low Z elements are comparatively more important for the study of astrophysical plasmas, the heavier ones are of more interest in laboratory sources. Of particular interest are ions of the fifth row elements, because these are increasingly injected as impurities in tokamak fusion plasmas. Considerable attention has been paid to calculations of atomic data for low Z elements, such as energy levels and radiative decay rates – see for example [3, 4]. However, similar atomic data are (generally) lacking for heavier ions, although Sampson et al. [5] have performed calculations for a wide range of F-like ions with $22 \leq Z \leq 92$ by using their Dirac-Fock-Slater (DFS) code. Their focus was on collisional data, but they also reported oscillator strengths for electric dipole transitions, although only from the lowest three levels of the $2s^22p^5$ and $2s2p^6$ configurations to the 110 excited levels of $2s^22p^43\ell$, $2s2p^53\ell$ and $2p^63\ell$. Furthermore, they did not report energy levels, although these can be inferred from their tabulations of collision strengths, but only for a few ions, as for brevity they did not report data for all. Similarly, Jönsson et al. [6] have calculated energies and radiative rates (A-values) for a wide range of ions with $14 \leq Z \leq 74$. They adopted the general-purpose relativistic atomic structure package (GRASP) code [7] and have included very large configuration interaction (CI) for the calculations. However, their results are restricted to the lowest 3 levels of the $2s^22p^5$ and $2s2p^6$ configurations. For the same transitions, measurements for wavelengths have also been made in laser-produced plasmas for many F-like ions, i.e. $38 \leq Z \leq 50$ [1, 2, 8–10]. Additionally, Zigler et al. [11] have identified 11 lines in the 6–7 Å range of the $(2s^22p^5)^2p – (2s^22p^4)^3s, 3d$ transitions of Rb XXIX. However, for modelling applications a larger set of data are (preferably) required. With this in mind and the requirements for the developing ITER project, we have already reported energy levels and A-values for two ions, namely Kr XXVIII [12] and Xe XLVI [13], and here we calculate similar data for all F-like ions with $37 \leq Z \leq 53$.

As in our earlier work [12, 13], we adopt the GRASP code for our calculations, and for the optimisation of the orbitals use the option of ‘extended average level’ (EAL), in which a weighted (proportional to $2j+1$) trace of the Hamiltonian matrix is minimised. However, our version of the code is slightly different from the one used by Jönsson et al. [6], although all versions originate from the same source [14] and provide similar results. This version has been revised by one of
the authors (P. H. Norrington), is referred to as GRASP0 and is freely available at http://web.am.qub.ac.uk/DARC/.

As in our earlier work for Kr and Xe ions, we report energies for the lowest 113 levels of the $2s^22p^5$, $2s2p^6$, $2s^22p^4\ell$, $2s2p^5\ell$, and $2p^6\ell$ configurations, although calculations have been performed for a much larger number of levels – see section 2. Similarly, we list A-values for all transitions among these levels for four types, namely electric dipole (E1), magnetic dipole (M1), electric quadrupole (E2), and magnetic quadrupole (M2). These results are required for the further calculation of lifetimes.

2. Energy levels

In our earlier work [12, 13], CI was included among the basic 11 configurations, i.e $2s^22p^5$, $2s2p^6$, $2s^22p^4\ell$, $2s2p^5\ell$, and $2p^6\ell$, which generate a total of 113 levels. However, in the present paper we include an additional 27 configurations, which are: $2s^22p^4\ell$, $2s2p^5\ell$, $2p^6\ell$, $2s^22p^45\ell$, $2s2p^55\ell$, and $2p^65\ell$. These 38 configurations generate 501 levels in total and provide slightly more accurate results than those obtained with the basic 11. Energies for the lowest 113 levels, obtained with the inclusion of Breit and quantum electrodynamic effects, are listed in Tables 1–17 for ions with $37 \leq Z \leq 53$. We note that energies of the higher levels from other configurations lie above the listed 113 and there is no mixing for any ion considered here.

For any calculation it is very important to assess accuracy so that results can be confidently applied in plasma modelling [15]. It is generally easier to assess the accuracy of energy levels if corresponding experimental data are available. Unfortunately, that is not the case for a majority of the levels for the ions studied here, although a few measurements are available, such as by [1, 2, 8–11] as already noted. The available experimental data have been assessed by the National Institute of Standards and Technology (NIST) personnel and their compiled results are available at the website http://www.nist.gov/pml/data/asd.cfm.

Another method of assessing accuracy is to perform calculations by a different and independent approach. For this we have adopted the Flexible Atomic Code (FAC) of Gu [16]. This is also a fully relativistic code and is available from the website https://www-amdis.iaea.org/FAC/. The advantages of FAC are that it is highly efficient to run and generally yields results comparable to those obtained with other atomic structure codes, as has already been demonstrated in several of our earlier papers, including those on F-like Kr XXVIII [12] and Xe XLVI [13]. Therefore, the results obtained (FAC1) with the same CI as with GRASP are also listed in Tables 1–17. Both sets of energies, for all ions, agree very well (within 0.05 Ryd) and there is no serious discrepancy in level orderings. However, this result is fully expected and therefore not very useful for assessing the accuracy. For some ions, the inclusion of a very large CI helps to improve the accuracy of the energy levels, as already noted in our earlier work [12, 13]. We have hence performed another calculation (FAC2) with 38 089 levels. The levels additional to those of FAC1 arise from all possible combinations of the $(2*5) 3*2, 4*2, 5*2, 3*1 4*1, 3*1 5*1, and 4*1 5*1$ configurations. These results are also listed in Tables 1–17, but we discuss in detail, as an example, level energies for only Sr XXX.

In comparison to FAC1, the energies from the FAC2 calculations are lower by up to 0.17 Ryd ($\leq 0.1\%$) for many levels, but there is no (major) discrepancy in level orderings. More importantly, the FAC2 energies are consistently lower for all levels and therefore are assessed to be comparatively more accurate. Since the effect of the additional CI included in FAC2 is noticeable, this may increase with yet more CI. Therefore, we have performed another calculation (FAC3) by almost doubling the number of levels, specifically by including 72 259 levels in total, the additional ones arising from
the \((2^6)\) 6\(^*\)1, 7\(^*\)1, 8\(^*\)1 and \((2^5\ 3^1)\) 6\(^*\)1, 7\(^*\)1, and 8\(^*\)1 configurations. The energies obtained for the lowest 113 levels of Sr XXX from these FAC3 calculations are also listed in Table 2. However, the differences between the FAC2 and FAC3 energies are insignificant \((\leq 0.013 \text{ Ryd})\). For many levels the FAC3 energies are lower than those from FAC2 but for a few the reverse is true – see for example, 6, 14 and 18. Therefore, we can confidently state that energies for the lowest 113 levels of Sr XXX (and other ions) have converged and the CI included in the FAC2 calculations is sufficient to obtain accurate results.

A major problem for most atomic structure calculations is the identification of level designations. Although levels of higher configurations do not mix with the lowest 113 of the F-like ions considered here, there is considerable mixing among themselves for a few. As an example, we list in Table A all the levels of Sr XXX which are highly mixed. For this reason the level designations provided in Tables 1–17 should not be taken as definitive, as a few may (inter)change depending on the calculation with different codes and/or CI. We have attempted to identify the levels based on the strength of their eigenvectors, but for a few ambiguity remains, such as 6/38, 8/26 and 24/31. This is because in such cases a single eigenvector of a configuration state function (CSF) dominates in several levels.

As already stated, experimental energies for some levels are available on the NIST website for a few ions, namely Rb XXIX, Sr XXX and Mo XXXIV. Energy levels for Sr XXX have already been compared with theoretical results [17], which are similar to our calculations. Therefore, in Tables B and C we compare our results with those of NIST for the common levels of Rb XXIX and Mo XXXIV, respectively. The NIST energy levels for Rb XXIX have been compiled by Sansonetti [18] and generally agree with our calculations, although differences for a few are up to 0.4 Ryd – see for example levels 36, 51, 53, and 66 in Table B. There is no trend, because for some our energies are higher and for a few lower. Additionally, there are some differences in the level designations and for this reason we have included mixing coefficients for these levels plus a few other which will help to explain the reason. As an example, level 40 is designated as \(2s^22p^4(^3P)^4F_{5/2}\) (45 in Table B) by NIST but is \(2s^22p^4(^1S)3d\ 2D_{5/2}\) in our work. Level 40 is well mixed with 45 and hence their labels can be interchanged, whereas 45 has a clear dominance of \(\sim 48\%\). Similar differences in the designations are found for levels 38/46, 39/66 and 43/66.

Energies for a few levels for Mo XXXIV have been compiled by Sugar and Musgrove [19] and are included in Table C along with our corresponding results from GRASP. The differences for a few levels are up to 0.45 Ryd (0.2\%), particularly for level 43, i.e. \(2s^22p^4^3d\ 4F_{3/2}\). Additionally, as for the levels of Rb XXIX in Table B, for Mo XXXIV there are some differences in label designations between our results and NIST. The change of labels are for 30/46, 31/72, 43/72, and 45/46, and for this reason we have provided mixing coefficients for these levels in Table C. Apart from these, many more levels are highly mixed and therefore there are always differences in the level designations between any two independent studies.

Finally, as stated earlier, Jönsson et al. [6] have reported energies for the \(2s^22p^5\ 2P_{1/2}\) and \(2s2p^6\ 2S_{1/2}\) levels of many ions, and in Table D we compare their plus available experimental results with our calculations with both GRASP and FAC. It is clear that, in general, the theoretical energies of Jönsson et al. [6] are closer to the experimental ones, whereas our calculated energies with both codes are consistently lower by \(\sim 0.02 \text{ Ryd}\) for the level \(2s^22p^5\ 2P_{1/2}\) and \(\sim 0.2 \text{ Ryd}\) higher for \(2s2p^6\ 2S_{1/2}\). This is because Jönsson et al. have performed very large calculations by including up to 73 000 and 15 000 CSFs for the respective levels, whereas our calculations are comparatively modest keeping in mind the larger number of levels considered in the work. However, it is interesting to note that for a few ions our calculated energies are
slightly closer to the measurements – see for example $Z = 39$ and 41 for $2s^2 2p^5 \, {}^2P_{1/2}$ and $Z = 50$ for $2s2p^6 \, {}^2S_{1/2}$. To conclude, based on the comparisons shown in Tables B, C and D we may confidently state that our energy levels listed in Tables 1–17 are accurate to $\sim$0.5%.

3. Radiative rates

In Tables 18–34 we present our calculated results with the GRASP code for energies (wavelengths, $\lambda_{ji}$ in Å), radiative rates ($A$-values, in s$^{-1}$), oscillator strengths ($f$-values, dimensionless), and line strengths ($S$-values, in atomic units, 1 a.u. = $6.460 \times 10^{-36}$ cm$^2$ esu$^2$) for E1 transitions in F-like ions with $37 \leq Z \leq 53$. However, for E2, M1 and M2 transitions only the $A$-values are listed, because the corresponding results for $f$- or $S$-values can be obtained using Eqs. (1-5) given in [12]. Additionally, we list the ratio ($R$) of the velocity (Coulomb gauge) and length (Babushkin gauge) forms which generally give an indication of the accuracy. The indices used to represent the lower and upper levels of a transition are defined in Tables 1–17. Furthermore, for brevity only transitions from the lowest 3 to higher excited levels are listed in Tables 18–34, but full tables are available online in the electronic version.

Jönsson et al. [6] have reported $A$-values for transitions among the lowest 3 levels of F-like ions, and in Table E we compare our results for the 1–3 E1, 2–3 E1, 1–2 M1, and 1–2 E2 transitions. There is no discrepancy for any transition and/or ion and all results agree to better than 5%. This is highly satisfactory and to a certain extent confirms the accuracy of our results. However, this comparison is very limited and therefore in Table F we compare our $f$-values for three ions, namely Mo XXXIV, Pd XXXVIII and Sn XLII with the earlier work of Sampson et al. [5], for all E1 transitions from the ground level. Since the level orderings are not the same for all ions, the upper level $J$ is also listed in this table which corresponds to Tables 6, 10 and 14 for the respective ions. For most transitions with significant $f$-values ($f \geq 0.01$) there is no discrepancy and both calculations agree within $\sim$10%. However, for some weaker transitions the differences between the two sets of $f$-values are sizeable – see for example, 1–97/98 of Mo XXXIV, 1–90/97 of Pd XXXVIII and 1–73/97 of Sn XLII. This is because the weaker transitions are more susceptible to change with differing amount of CI and/or methods.

Finally, we discuss the ratio ($R$) of the velocity and length forms of the $f$-value to further assess the accuracy. For brevity, we only discuss results for transitions in Sr XXX, although the same conclusions apply to all ions considered here. Among the lowest 113 levels, there are 2191 possible E1 transitions, of which 385 have $f \geq 0.01$, i.e. they are comparatively strong. For most of these 385 transitions, $R$ is within 20% of unity, although for about 25% (104), $R$ is up to a factor of 2 (such as 96–106, $f = 0.020$ and 105–113, $f = 0.026$), and only for one (58–106; $f = 0.011$) is $R = 3$. Furthermore, all such transitions have $f < 0.1$. However, for a few very weak transitions, $R$ is up to several orders of magnitude, and examples include 5–111 ($f \sim 3 \times 10^{-7}$), 14–43 ($f \sim 4 \times 10^{-5}$) and 25–26 ($f \sim 6 \times 10^{-9}$). As already stated, $f$-values for such weak transitions are highly variable with differing amount of CI, because of the cancellation and/or additive effects of different matrix elements, and hence are comparatively less reliable. However, due to their small magnitudes, their contribution to the modelling of plasmas is normally expected to be small. Overall, based on this and other comparisons already discussed, our assessment of accuracy for the $f$- (and $A$-) values for a majority of strong transitions is $\sim$20%, for all ions.
4. Lifetimes

Once the A-values are known, the lifetime $\tau$ of a level $j$ can be easily determined as $1.0/\Sigma_i A_{ji}$, where the summation includes results from all types of transitions, i.e. E1, E2, M1, and M2. Since this is a measurable quantity it helps to assess the accuracy of radiative rates, particularly when a single A-value for any type of transition dominates. To our knowledge no measurements of $\tau$ are available for the levels of the F-like ions considered here, but in Tables 1–17 we have listed our calculated results for future comparisons and assessment of accuracy. Previous theoretical results are available for only one ion, namely Sr XXX [17], for which there is discrepancy for only level 2, i.e. $2s^22p^5\,^2P_{1/2}^o$, and the $\tau$ of [17] is underestimated by a factor of 2 as already explained [20].

5. Conclusions

Energies for the lowest 113 levels of the $2s^22p^5$, $2s2p^6$, $2s^22p^43\ell$, $2s2p^53\ell$, and $2p^63\ell$ configurations of 17 F-like ions with $37 \leq Z \leq 53$ are reported. For the calculations the GRASP code has been adopted, although for an accuracy assessment the FAC is also employed with much more extensive CI. Based on several calculations with both codes and comparisons with available theoretical and experimental data, our energy levels are assessed to be accurate to better than 0.5%, for all ions. However, for a few levels of each ion there is some ambiguity in level designations, because of very strong mixing with often one eigenvector of a CSF dominating in magnitude for several levels.

Radiative rates for E1, E2, M1, and M2 transitions are also reported among the lowest 113 levels, and our data are significantly more extensive than currently available in the literature. However, there is no major discrepancy for any transition and/or ion. Based on several comparisons with different calculations, the accuracy of our A-values is assessed to be $\sim 20\%$, particularly for strong transitions with large f-values, although for very weak transitions the reported A-values may be comparatively less reliable.

For future comparisons, lifetimes for these levels are also listed although no measurements are currently available in the literature. However, previous theoretical values are available for the levels of Sr XXX, and there is no discrepancy with our work, except for one level. Finally, calculations for energies have been made for up to 38 089 levels and for A-values among 501 levels, for all ions. Therefore, a larger set of data than presented here for any ion may be obtained on request from the first author (K.Aggarwal@qub.ac.uk).

Acknowledgments

KMA is thankful to AWE Aldermaston for financial support.

Appendix A. Supplementary data

Owing to space limitations, only parts of Tables 18–34 are presented here, but full tables are being made available as supplemental material in conjunction with the electronic publication of this work. Supplementary data associated with this article can be found, in the online version, at doi:nn.mnn/j.adt.2016.nn.nnn.
References

[1] J. Reader, Phys. Rev. 26 (1982) 501.
[2] J. Reader, C.M. Brown, J.O. Ekberg, U. Feldman, J.F. Seely, W.E. Behring, J. Opt. Soc. Am. B3 (1986) 1609.
[3] H.M.S. Blackford, A. Hibbert, At. Data Nucl. Data Tables 58 (1994) 101.
[4] C. Froese Fischer, G. Tachiev, At. Data Nucl. Data Tables 87 (2004) 1.
[5] D.H. Sampson, H.L. Zhang, C.J. Fontes, At. Data Nucl. Data Tables 48 (1991) 25.
[6] P. Jönsson, A. Alkauskas, G. Gaigalas, At. Data Nucl. Data Tables 99 (2013) 431.
[7] P. Jönsson, X. He, C.F. Fischer, I.P. Grant, Comput. Phys. Commun. 177 (2007) 597.
[8] R.J. Hutcheon, L. Cooke, M.H. Key, C.L.S. Lewis, G.E. Bromage, Phys. Scr. 21 (1980) 89.
[9] U. Feldman, J.F. Seely, W.E. Behring, M.C. Richardson, S. Goldsmith, J. Opt. Soc. Am. B2 (1985) 1658.
[10] U. Feldman, J.O. Ekberg, J.F. Seely, C.M. Brown, D.R. Kania, B.J. MacGowan, C.J. Keane, W.E. Behring, J. Opt. Soc. Am. B8 (1991) 531.
[11] A. Zigler, U. Feldman, G.A. Doschek, J. Opt. Soc. Am. B3 (1986) 1221.
[12] K.M. Aggarwal, F.P. Keenan, K.D. Lawson, At. Data Nucl. Data Tables 94 (2008) 323.
[13] K.M. Aggarwal, F.P. Keenan, K.D. Lawson, At. Data Nucl. Data Tables 96 (2010) 123.
[14] I.P. Grant, B.J. McKenzie, P.H. Norrington, D.F. Mayers, N.C. Pyper, Comput. Phys. Commun. 21 (1980) 207.
[15] K.M. Aggarwal, F.P. Keenan, Fusion Sci. Tech. 63 (2013) 363.
[16] M.F. Gu, Can. J. Phys. 86 (2008) 675.
[17] A. Goyal, I. Khatri, S. Aggarwal, A.K. Singh, M. Mohan, J. Quant. Spect. Rad. Transf. 161 (2015) 157.
[18] J.E. Sansonetti, J. Phys. Chem. Ref. Data 35 (2006) 301.
[19] J. Sugar, A. Musgrove, J. Phys. Chem. Ref. Data 17 (1988) 155.
[20] K.M. Aggarwal, J. Quant. Spect. Rad. Transf. 166 (2015) 108.
Table A
Mixing coefficients (MC) for some levels of Sr XXX. Numbers outside and inside a bracket correspond to MC and the level, respectively. See Table 2 for the definition of all levels.

| Index | Configuration | Level | Mixing coefficients |
|-------|---------------|-------|---------------------|
| 1     | 2s<sup>2</sup>2p<sup>4</sup>4s | 2S<sub>/2</sub> | 0.60(38)-0.36(13)+0.71(6) |
| 2     | 2s<sup>2</sup>2p<sup>4</sup>(3P)<sub>3p</sub> | 2D<sub>/2</sub> | 0.56(26)-0.47(11)+0.49(8)+0.40(22)-0.25(37) |
| 3     | 2s<sup>2</sup>2p<sup>4</sup>3p | 4D<sub>/2</sub> | 0.54(14)+0.55(29)-0.29(41)+0.57(49) |
| 4     | 2s<sup>2</sup>2p<sup>4</sup>(3P)<sub>3p</sub> | 2P<sub>/2</sub> | 0.55(20)+0.38(7)-0.25(18)-0.21(35)+0.65(56) |
| 5     | 2s<sup>2</sup>2p<sup>4</sup>3d | 4D<sub>/2</sub> | -0.64(21)+0.46(33)-0.27(66)+0.20(47)+0.20(58)-0.25(53) |
| 6     | 2s<sup>2</sup>2p<sup>4</sup>3d | 4P<sub>/2</sub> | 0.47(42)-0.56(24)-0.45(31)+0.50(59) |
| 7     | 2s<sup>2</sup>2p<sup>4</sup>3p | 4D<sub>/2</sub> | 0.76(20)+0.50(11)-0.38(8) |
| 8     | 2s<sup>2</sup>2p<sup>4</sup>(1P)<sub>3d</sub> | 2P<sub>/2</sub> | 0.63(24)-0.57(31)+0.47(54) |
| 9     | 2s<sup>2</sup>2p<sup>4</sup>4s | 2D<sub>/2</sub> | -0.57(38)+0.44(13)+0.68(6) |
| 10    | 2s<sup>2</sup>2p<sup>4</sup>(1S)<sub>3d</sub> | 2D<sub>/2</sub> | 0.56(43)+0.47(47)+0.21(58)+0.59(39) |
| 11    | 2s<sup>2</sup>2p<sup>4</sup>3d | 4F<sub>/2</sub> | 0.50(45)+0.34(23)+0.22(40)-0.27(36)+0.67(65) |
| 12    | 2s<sup>2</sup>2p<sup>4</sup>(1S)<sub>3d</sub> | 2F<sub>/2</sub> | -0.45(43)+0.63(21)+0.38(33)-0.25(66)+0.29(47)+0.26(58) |
| 13    | 2s<sup>2</sup>2p<sup>4</sup>3d | 4P<sub>/2</sub> | -0.44(14)-0.52(10)-0.22(29)+0.65(49) |
| 14    | 2s<sup>2</sup>2p<sup>4</sup>(3P)<sub>3p</sub> | 2P<sub>/2</sub> | -0.37(20)-0.34(7)-0.26(17)-0.40(30)+0.68(56) |
| 15    | 2s<sup>2</sup>2p<sup>4</sup>(3P)<sub>3p</sub> | 2D<sub>/2</sub> | 0.67(74)-0.42(69)+0.61(64) |
| 16    | 2s<sup>2</sup>2p<sup>4</sup>(1S)<sub>3d</sub> | 2D<sub>/2</sub> | -0.33(45)-0.33(23)-0.33(40)-0.39(46)+0.69(65) |
| 17    | 2s<sup>2</sup>2p<sup>4</sup>(1P)<sub>3d</sub> | 2D<sub>/2</sub> | -0.44(43)-0.28(21)-0.40(66)-0.33(47)+0.66(39) |
| 18    | 2s<sup>2</sup>2p<sup>4</sup>3p | 4D<sub>/2</sub> | -0.45(68)+0.50(63)-0.37(75)+0.61(72) |
| 19    | 2s<sup>2</sup>2p<sup>4</sup>3p | 4P<sub>/2</sub> | 0.51(80)-0.67(71)-0.23(73)+0.39(96)-0.28(98) |
| 20    | 2s<sup>2</sup>2p<sup>4</sup>(3P)<sub>3p</sub> | 2P<sub>/2</sub> | -0.54(68)-0.66(72)+0.46(89) |
| 21    | 2s<sup>2</sup>2p<sup>4</sup>3p | 4D<sub>/2</sub> | -0.61(74)-0.46(69)+0.37(64)+0.52(97) |
| 22    | 2s<sup>2</sup>2p<sup>4</sup>(3P)<sub>3p</sub> | 2S<sub>/2</sub> | 0.51(80)+0.62(71)-0.37(77)+0.36(96)+0.23(98) |
| 23    | 2s<sup>2</sup>2p<sup>4</sup>3d | 4F<sub>/2</sub> | -0.41(92)+0.71(83)-0.56(101) |
| 24    | 2s<sup>2</sup>2p<sup>4</sup>(1P)<sub>3d</sub> | 2D<sub>/2</sub> | -0.45(92)+0.46(101)-0.38(95)+0.65(85) |
| 25    | 2s<sup>2</sup>2p<sup>4</sup>(1P)<sub>3d</sub> | 2D<sub>/2</sub> | 0.46(102)-0.36(93)-0.28(81)-0.63(88)+0.36(100)+0.21(108) |
| 26    | 2s<sup>2</sup>2p<sup>4</sup>3d | 4D<sub>/2</sub> | 0.68(90)-0.71(91) |
| 27    | 2s<sup>2</sup>2p<sup>4</sup>(1P)<sub>3d</sub> | 2P<sub>/2</sub> | 0.54(90)+0.60(91)+0.58(106) |
| 28    | 2s<sup>2</sup>2p<sup>4</sup>3d | 4P<sub>/2</sub> | -0.51(92)-0.24(83)-0.24(95)-0.59(85)+0.52(103) |
| 29    | 2s<sup>2</sup>2p<sup>4</sup>3d | 4D<sub>/2</sub> | 0.33(102)-0.44(93)-0.26(81)+0.46(88)-0.40(100)+0.29(108)-0.43(105) |
| 30    | 2s<sup>2</sup>2p<sup>4</sup>3d | 4P<sub>/2</sub> | -0.50(84)-0.51(94)+0.47(87)+0.52(104) |
| 31    | 2s<sup>2</sup>2p<sup>4</sup>(1P)<sub>3d</sub> | 2P<sub>/2</sub> | -0.44(92)-0.54(83)-0.41(101)+0.49(95)+0.28(85) |
| 32    | 2s<sup>2</sup>2p<sup>4</sup>(1P)<sub>3d</sub> | 2P<sub>/2</sub> | 0.36(84)+0.31(94)-0.21(87)+0.85(104) |
### Table B

Comparison of some energy levels of Rb XXIX (in Ryd) and their mixing coefficients (MC). Numbers outside and inside a bracket correspond to MC and the level, respectively. See Table 1 for definition of all levels.

| Index | Configuration | Level | NIST | GRASP | Mixing coefficients |
|-------|---------------|-------|------|-------|----------------------|
| 1     | 2s²2p⁵        | ²P₀/² | 0.000  | 0.0000 | 1.00 (1)             |
| 2     | 2s²2p⁵        | ²P₁/² | 4.596  | 4.5872 | 1.00 (2)             |
| 3     | 2s²2p⁶        | ²S₁/₂ | 18.325 | 18.4716| 1.00 (3)             |
| 4     | 2s²2p¹3s      | ²P₁/₂ | 135.186 | 135.0347| 0.40 (9)+0.77 (5)+0.49 (16) |
| 5     | 2s²2p¹3s      | ²D₅/₂ | 140.153 | 140.0749| 0.46 (4)+0.89 (15)   |
| 36    | 2s²2p¹3d      | ²P₃/₂ | 145.775 | 145.3680| -0.58 (36)-0.52 (66)+0.27 (57)+0.35 (54)+0.37 (39) |
| 38    | 2s²2p¹(3P)³d  | ²D₅/₂ | 145.6587| 0.48 (64)-0.47 (46)+0.53 (38)+0.35 (56)+0.24 (53)+0.21 (40) |
| 39    | 2s²2p¹(1S)³d  | ²D₃/₂ | 146.1513| 0.57 (43)+0.46 (47)+0.20 (57)+0.59 (39) |
| 40    | 2s²2p¹(1S)³d  | ²D₃/₂ | 146.249 | 146.4424| 0.51 (45)+0.34 (24)+0.23 (64)+0.26 (38)+0.65 (40) |
| 43    | 2s²2p¹3d      | ²F₃/₂ | 148.855 | 148.7185| -0.44 (43)+0.63 (23)+0.39 (36)+0.26 (66)+0.29 (47)+0.27 (57) |
| 45    | 2s²2p¹3d      | ²F₅/₂ | 149.1016| 0.69 (45)-0.38 (64)+0.49 (38)+0.24 (56)+0.21 (53) |
| 46    | 2s²2p¹(3P)³d  | ²F₅/₂ | 149.220 | 149.2505| 0.26 (24)+0.52 (64)+0.76 (46)+0.22 (38) |
| 51    | 2s²2p¹(1D)³d  | ²S₁/₂ | 150.323 | 150.0290| -0.47 (27)+0.35 (59)+0.81 (51) |
| 53    | 2s²2p¹(1D)³d  | ²D₅/₂ | 150.496 | 150.0662| 0.27 (64)+0.24 (38)-0.45 (56)-0.77 (53) |
| 54    | 2s²2p¹(1D)³d  | ²P₃/₂ | 150.396 | 150.2640| -0.28 (43)+0.36 (36)+0.32 (47)+0.22 (57)+0.76 (54) |
| 57    | 2s²2p¹(1D)³d  | ²D₃/₂ | 150.769 | 151.0617| 0.22 (43)-0.54 (66)-0.75 (57) |
| 66    | 2s²2p¹(3P)³d  | ²D₃/₂ | 155.690 | 155.2074| -0.43 (43)-0.23 (23)-0.40 (66)-0.53 (47)+0.67 (39) |

NIST: [http://www.nist.gov/pml/data/asd.cfm](http://www.nist.gov/pml/data/asd.cfm)
GRASP: Present results with the GRASP code with 501 level calculations

### Table C

Comparison of some energy levels of Mo XXXIV (in Ryd) and their mixing coefficients (MC). Numbers outside and inside a bracket correspond to MC and the level, respectively. See Table 6 for definition of all levels.

| Index | Configuration | Level | NIST | GRASP | Mixing coefficients |
|-------|---------------|-------|------|-------|----------------------|
| 1     | 2s²2p⁵        | ²P₀/² | 0.0000 | 0.0000 | 1.00 (1)             |
| 2     | 2s²2p⁵        | ²P₁/² | 8.0766 | 8.0624 | 1.00 (2)             |
| 3     | 2s²2p⁶        | ²S₁/₂ | 24.1969| 24.3494| 1.00 (3)             |
| 30    | 2s²2p¹(3P)³d  | ²D₅/₂ | 194.6613| 0.47 (71)-0.45 (46)+0.53 (30)+0.36 (53)+0.30 (51)+0.22 (35) |
| 31    | 2s²2p¹(1S)³d  | ²D₃/₂ | 195.1778| 0.50 (43)+0.40 (47)+0.24 (58)+0.58 (31) |
| 43    | 2s²2p¹3d      | ²F₃/₂ | 200.2783| 200.7266| -0.49 (43)+0.62 (19)+0.36 (28)-0.21 (72)+0.31 (47)+0.25 (58) |
| 45    | 2s²2p¹3d      | ²F₅/₂ | 200.8979| 201.3380| 0.74 (45)-0.21 (71)+0.27 (46)+0.49 (30)+0.26 (53) |
| 46    | 2s²2p¹(1P)³d  | ²F₃/₂ | 201.5632| 201.4998| 0.32 (20)+0.60 (71)+0.72 (46) |
| 50    | 2s²2p¹(1D)³d  | ²S₁/₂ | 201.9641| 202.2953| -0.51 (21)-0.39 (59)+0.76 (50) |
| 51    | 2s²2p¹(1D)³d  | ²D₅/₂ | 202.3651| 202.3860| -0.26 (20)+0.33 (71)-0.29 (53)-0.82 (51) |
| 52    | 2s²2p¹(1D)³d  | ²P₁/₂ | 202.2375| 202.4757| -0.27 (43)-0.21 (19)+0.41 (28)+0.31 (47)-0.31 (58)+0.71 (52) |
| 53    | 2s²2p¹(1D)³d  | ²F₃/₂ | 202.2375| 202.5446| 0.28 (20)+0.51 (30)-0.76 (53)+0.26 (51) |
| 58    | 2s²2p¹(1D)³d  | ²D₃/₂ | 203.4039| 203.5764| 0.25 (43)-0.58 (72)-0.71 (58)-0.23 (52) |
| 59    | 2s²2p¹(1D)³d  | ²P₁/₂ | 203.7684| 203.8744| -0.60 (27)-0.70 (59)-0.38 (50) |
| 72    | 2s²2p¹(1P)³d  | ²D₃/₂ | 210.8945| 211.0131| -0.47 (43)-0.26 (19)-0.39 (72)-0.33 (47)+0.64 (31) |

NIST: [http://www.nist.gov/pml/data/asd.cfm](http://www.nist.gov/pml/data/asd.cfm)
GRASP: Present results with the GRASP code with 501 level calculations
Table D
Comparison of energy levels of ions with $37 \leq Z \leq 53$ (in Ryd).

| Z  | Experimental | GRASP\textsubscript{a} | GRASP\textsubscript{b} | FAC |
|----|--------------|----------------------|----------------------|-----|
|    | $2s^22p^1P^0_{1/2}$ | $2s^22p^1S^0_{1/2}$ | $2s^22p^1P^0_{1/2}$ | $2s^22p^1S^0_{1/2}$ | $2s^22p^1P^0_{1/2}$ | $2s^22p^1S^0_{1/2}$ |
| 37 | 4.5962       | 18.3250              | 4.5967               | 18.3236 | 4.5872 | 18.4716 | 4.5881 | 18.4550 |
| 38 | 5.1793       | 19.3763              | 5.1765               | 19.3736 | 5.1663 | 19.5230 | 5.1676 | 19.5061 |
| 39 | 5.8072       | 20.4798              | 5.8106               | 20.4818 | 5.7998 | 20.6264 | 5.8014 | 20.6156 |
| 40 | 6.5001       | 21.6581              | 6.5028               | 21.6520 | 6.4911 | 21.8044 | 6.4932 | 21.7870 |
| 41 | 7.2500       | 22.8765              | 7.2565               | 22.8879 | 7.2441 | 23.0419 | 7.2466 | 23.0244 |
| 42 | 8.0756       | 24.1969              | 8.0756               | 24.1035 | 8.0624 | 24.3494 | 8.0655 | 24.3315 |
| 43 | 8.9641       | 25.5730              | 8.9500               | 25.7308 | 8.9538 | 25.7127 |
| 44 | 9.9262       | 27.0306              | 9.9112               | 27.3906 | 9.9157 | 27.1721 |
| 45 | 10.9753      | 28.5874              | 10.9661              | 28.5709 | 10.9520 | 28.7331 | 10.9555 | 28.7143 |
| 46 | 12.0883      | 30.1983              | 12.0715              | 30.3631 | 12.0777 | 30.3438 |
| 47 | 31.9272      | 31.9179              | 31.9179              | 31.9797 | 32.0854 | 13.2869 | 32.0656 |
| 48 | 33.7734      | 33.7344              | 33.7344              | 33.7977 | 33.9050 | 14.5880 | 33.8845 |
| 49 | 15.9964      | 35.6533              | 15.9764              | 35.8272 | 15.9860 | 35.8059 |
| 50 | 37.7137      | 37.6799              | 37.6799              | 37.8574 | 37.8852 | 37.8351 |
| 51 | 19.1037      | 39.8195              | 19.0815              | 40.0012 | 19.0909 | 39.9778 |
| 52 | 20.8243      | 42.0784              | 20.8009              | 42.2645 | 20.8149 | 42.2395 |
| 53 | 22.6639      | 44.4631              | 22.6393              | 44.6534 | 22.6550 | 44.6272 |

Experimental: see Jönsson et al. [6]
GRASP\textsubscript{a}: earlier calculations of Jönsson et al. [6] with the GRASP code
GRASP\textsubscript{b}: present calculations with the GRASP code for 501 levels
FAC: present calculations with the FAC code for 38 089 levels
Table E
Comparison of A-values (s$^{-1}$) for transitions among the lowest three levels of ions with $37 \leq Z \leq 53$. The first entry is from the present calculations with GRASP and the second is from Jönsson et al. [6]. $a \pm b \equiv a \times 10^{\pm b}$.

| Z  | 1–3 (E1)  | 2–3 (E1)  | 1–2 (M1)  | 1–2 (E2)  |
|----|-----------|-----------|-----------|-----------|
| 37 | 2.521+11  | 5.171+10  | 2.274+06  | 1.054+03  |
| 37 | 2.419+11  | 4.911+10  | 2.289+06  | 1.051+03  |
| 38 | 2.806+11  | 5.379+10  | 3.247+06  | 1.687+03  |
| 38 | 2.698+11  | 5.116+10  | 3.266+06  | 1.681+03  |
| 39 | 3.128+11  | 5.591+10  | 4.591+06  | 2.665+03  |
| 39 | 3.012+11  | 5.232+10  | 4.617+06  | 2.656+03  |
| 40 | 3.492+11  | 5.806+10  | 6.492+06  | 4.159+03  |
| 40 | 3.367+11  | 5.534+10  | 6.468+06  | 4.146+03  |
| 41 | 3.903+11  | 6.024+10  | 8.933+06  | 6.419+03  |
| 41 | 3.678+11  | 5.747+10  | 8.981+06  | 6.399+03  |
| 42 | 4.367+11  | 6.246+10  | 1.231+07  | 9.800+03  |
| 42 | 4.222+11  | 5.964+10  | 1.237+07  | 9.770+03  |
| 43 | 4.894+11  | 6.472+10  | 1.683+07  | 1.481+04  |
| 43 | 4.737+11  | 6.185+10  | 1.691+07  | 1.477+04  |
| 44 | 5.490+11  | 6.701+10  | 2.283+07  | 2.217+04  |
| 44 | 5.320+11  | 6.409+10  | 2.294+07  | 2.210+04  |
| 45 | 6.165+11  | 6.935+10  | 3.077+07  | 3.288+04  |
| 45 | 5.981+11  | 6.637+10  | 3.091+07  | 3.278+04  |
| 46 | 6.931+11  | 7.172+10  | 4.110+07  | 4.834+04  |
| 46 | 6.731+11  | 6.868+10  | 4.137+07  | 4.819+04  |
| 47 | 7.800+11  | 7.415+10  | 5.479+07  | 7.047+04  |
| 47 | 7.582+11  | 7.104+10  | 5.503+07  | 7.027+04  |
| 48 | 8.786+11  | 7.661+10  | 7.245+07  | 1.019+05  |
| 48 | 8.548+11  | 7.344+10  | 7.275+07  | 1.016+05  |
| 49 | 9.906+11  | 7.913+10  | 9.524+07  | 1.463+05  |
| 49 | 9.645+11  | 7.587+10  | 9.563+07  | 1.459+05  |
| 50 | 1.118+12  | 8.169+10  | 1.245+08  | 2.086+05  |
| 50 | 1.089+12  | 7.836+10  | 1.250+08  | 2.080+05  |
| 51 | 1.262+12  | 8.430+10  | 1.620+08  | 2.952+05  |
| 51 | 1.231+12  | 8.088+10  | 1.636+08  | 2.944+05  |
| 52 | 1.420+12  | 8.697+10  | 2.066+08  | 4.150+05  |
| 52 | 1.391+12  | 8.346+10  | 2.104+08  | 4.139+05  |
| 53 | 1.612+12  | 8.969+10  | 2.700+08  | 5.799+05  |
| 53 | 1.574+12  | 8.609+10  | 2.709+08  | 5.783+05  |
Table F
Comparison of f-values (dimensionless) for transitions from the ground \((2s^22p^5\ 2P_{1/2})\) to higher excited levels of Mo XXXIV, Pd XXXVIII and Sn XLII. See Tables 6, 10 and 14 for definitions of J levels. \(a+b \equiv a \times 10^b\).

|   | Mo XXXIV | Pd XXXVIII | Sn XLII |
|---|---------|----------|---------|
|   | GRASP   | DFS      | GRASP   | DFS      | GRASP   | DFS      |
| 1 | 3       | 4.585−02 | 3       | 4.680−02 | 3       | 4.854−02 |
| 1 | 4       | 4.528−02 | 4       | 4.392−02 | 4       | 4.162−02 |
| 1 | 5       | 6.581−02 | 5       | 6.506−02 | 5       | 6.474−02 |
| 1 | 6       | 1.494−02 | 6       | 1.516−02 | 6       | 1.532−02 |
| 1 | 13      | 1.532−02 | 13      | 1.681−02 | 13      | 1.606−02 |
| 1 | 15      | 1.175−02 | 15      | 1.220−02 | 15      | 1.221−03 |
| 1 | 17      | 5.087−02 | 17      | 6.029−02 | 17      | 1.489−02 |
| 1 | 18      | 7.820−03 | 18      | 1.672−02 | 18      | 1.595−02 |
| 1 | 19      | 8.551−04 | 19      | 1.744−03 | 19      | 2.593−02 |
| 1 | 20      | 3.169−04 | 20      | 1.967−03 | 20      | 1.242−01 |
| 1 | 21      | 8.687−03 | 21      | 1.418−02 | 21      | 3.756−02 |
| 1 | 27      | 1.114−01 | 27      | 1.144−01 | 27      | 1.064−01 |
| 1 | 28      | 1.901−01 | 28      | 1.619−01 | 28      | 9.281−02 |
| 1 | 30      | 4.707−01 | 30      | 4.934−01 | 30      | 4.625−01 |
| 1 | 31      | 2.358−01 | 31      | 2.923−01 | 31      | 3.501−01 |
| 1 | 35      | 4.103−01 | 35      | 4.497−01 | 35      | 4.643−01 |
| 1 | 42      | 2.699−04 | 42      | 7.399−04 | 42      | 8.508−05 |
| 1 | 41      | 2.548−04 | 41      | 2.752−04 | 41      | 7.897−03 |
| 1 | 43      | 8.816−03 | 43      | 8.227−03 | 43      | 1.905−01 |
| 1 | 45      | 2.125−01 | 45      | 1.995−01 | 45      | 9.784−03 |
| 1 | 46      | 1.407−02 | 46      | 8.456−03 | 46      | 1.753−03 |
| 1 | 47      | 1.792−03 | 47      | 1.520−03 | 47      | 1.616−01 |
| 1 | 50      | 2.161−01 | 50      | 2.151−01 | 50      | 5.637−01 |
| 1 | 52      | 5.732−02 | 52      | 4.455−01 | 52      | 4.442−01 |
| 1 | 52      | 4.496−01 | 52      | 5.196−01 | 52      | 5.633−02 |
| 1 | 53      | 5.757−01 | 53      | 7.528−02 | 53      | 3.149−03 |
| 1 | 58      | 7.751−02 | 58      | 5.603−02 | 58      | 3.939−02 |
| 1 | 59      | 3.292−02 | 59      | 2.554−02 | 59      | 1.767−02 |
| 1 | 63      | 7.920−03 | 63      | 8.892−03 | 63      | 8.400−03 |
| 1 | 64      | 5.384−02 | 64      | 5.365−02 | 64      | 4.960−02 |
| 1 | 66      | 2.971−02 | 66      | 9.826−05 | 66      | 2.454−02 |
| 1 | 67      | 7.246−02 | 67      | 2.333−02 | 67      | 1.200−02 |
| 1 | 68      | 1.748−02 | 68      | 1.104−01 | 68      | 9.709−02 |
| 1 | 69      | 7.904−02 | 69      | 7.317−02 | 69      | 7.327−02 |
| 1 | 70      | 5.894−02 | 70      | 5.436−02 | 70      | 5.310−02 |
| 1 | 71      | 4.054−10 | 71      | 8.086−02 | 71      | 8.477−02 |
| 1 | 72      | 2.619−03 | 72      | 3.054−02 | 72      | 3.161−02 |
| 1 | 74      | 8.011−02 | 74      | 2.293−03 | 74      | 2.022−03 |
| 1 | 75      | 2.788−02 | 75      | 6.354−07 | 75      | 1.027−05 |
| 1 | 76      | 2.602−03 | 76      | 2.842−03 | 76      | 6.129−04 |
| 1 | 86      | 4.684−04 | 86      | 1.924−04 | 86      | 9.104−05 |
| 1 | 92      | 6.058−04 | 92      | 9.307−04 | 92      | 4.662−04 |
| 1 | 93      | 1.236−03 | 93      | 3.450−07 | 93      | 4.278−05 |
| 1 | 97      | 5.227−06 | 97      | 3.321−05 | 97      | 2.698−06 |
| 1 | 98      | 9.719−05 | 98      | 3.715−05 | 98      | 1.474−05 |
| 1 | 99      | 6.515−03 | 99      | 3.580−03 | 99      | 1.995−03 |
| 1 | 100     | 1.665−03 | 100     | 8.723−04 | 100     | 4.602−04 |
| 1 | 109     | 1.467−04 | 109     | 1.220−04 | 109     | 9.614−05 |
| 1 | 112     | 7.993−05 | 112     | 6.248−05 | 112     | 4.736−05 |
| 1 | 113     | 7.549−04 | 113     | 5.908−04 | 113     | 4.508−04 |

GRASP: present calculations with the GRASP code
DFS: earlier calculations of Sampson et al. [5] with the Dirac-Fock-Slater code