Predictive systematization of line strengths for the 2s²–2s2p resonance and intercombination transitions in the Be isoelectronic sequence

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Abstract. Measured lifetime data for the $2s^2 {}^1S_{0}-2s2p {}^{1.3}P_{1}$ resonance and intercombination lines in the Be isoelectronic sequence are critically evaluated, and jointly systematized using effective singlet–triplet-reduced line strengths S_r . The data are examined together with recent theoretical predictions in the linearizing exposition $Z^2S_r \cong S_H + B/(Z-C)$ and the high-Z trend is compared with the corresponding hydrogenic limit. Smoothed and interpolated predictions are presented for $Z \leq 54$.

1. Introduction

It has been observed [1-3] that atomic transition line strengths can often be represented for interpolation and critical evaluation by an empirical relationship

$$Z^{2}S = S_{\rm H} + B/(Z - C)$$
(1)

where *S* is the line strength, *Z* is the nuclear charge, and *S*_H, *B* and *C* are least-squares adjusted fitting constants. For $ns {}^{2}S_{1/2}$ – $np {}^{2}P_{J}$ resonance transitions in alkali-like isoelectronic sequences, it has been shown [4] that the fitted value for the parameter *S*_H matches the line strength for the corresponding transition in a hydrogen atom.

$$S_{\rm H} \Rightarrow \frac{3}{4}n^2(n^2-1)(2J+1)$$
. (2)

For $ns^{2-1}S_0$ – $nsnp^{-1.3}P_1$ transitions in alkaline-earth-like isoelectronic sequences, a formalism has been developed [5] through which intermediate coupling is characterized by a singlet–triplet mixing angle determined from spectroscopic energy level data. This approach permits the nominally ${}^{1}S_0{}^{-1}P_1$ resonance and ${}^{1}S_0{}^{-3}P_1$ intercombination transitions to be jointly systematized. This formalism has been applied to the $ns^2{}-nsnp$ transitions in the Be (n = 2) [5], Mg (n = 3) [5], Zn (n = 4) [6, 7], Cd (n = 5) [8] and Hg (n = 6)[8], sequences, and extended to the $2s^2{}-2s3p$ transitions in the Be sequence [9, 10]. Within the framework of 1/Z perturbation theory, it is clear that the unscreened hydrogenic line strength is also relevant to the high-Z limit of the alkaline-earth-like sequences, with two caveats. First, there may be effects due to the high-Z asymptotic degeneracy of levels in the same complex, which causes strong configuration mixing that is zeroth order in 1/Z, such as between $2s^2$ and $2p^2$ in the Be sequence. For alkali-like sequences, the hydrogenic value of $S_{\rm H}$ is independent of such asymptotic mixing, since levels of the same parity with different ℓ cannot have the same J. Second, the relativistic effects are more complicated in these two-electron spectra. For example the asymptotic degeneracy is now between $2s_{1/2}^2$

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and $2p_{1/2}^2$ only, and the Breit interaction should be included. However, these relativistic effects are not relevant to our analysis of the available data in the present case.

We report here an extension of the earlier preliminary study [5] of the Be-like $2s^2-2s2p$ transitions that includes a comprehensive and critical evaluation of the available lifetime data base, a comparison with recent theoretical calculations, an evaluation of the constant $S_{\rm H}$ using hydrogenic values with asymptotic configuration mixing, and data-based predictions for these lifetimes for $Z \leq 54$.

2. Calculational formulation

For an unbranched J = 0-1 transition, the line strength can be deduced from the upper level lifetime τ and the transition wavelength λ using

$$S = [\lambda(Å)/1265.38]^3 \ 3/\tau(ns) \,. \tag{3}$$

Theoretically, S is given to within angular factors by the square of the dipole transition moment. For the Be sequence, to first order in 1/Z the n = 2 intrashell transitions involve asymptotic configuration mixing in the J = 0 ground level and intermediate coupling in the J = 1 excited levels. Thus, except for the neutral end of the sequence, and subject to the caveats stated above, the non-relativistic wavefunctions can be written in terms of mixing angles ϕ and θ as

$$|\Psi_0\rangle = \cos\phi |2s^2 {}^1S_0\rangle + \sin\phi |2p^2 {}^1S_0\rangle$$
(4)

$$|\Psi_1\rangle = \cos\theta |2s2p \ ^1P_1\rangle - \sin\theta |2s2p \ ^3P_1\rangle$$
(5)

$$|\Psi_3\rangle = \sin\theta |2s2p \ ^1P_1\rangle + \cos\theta |2s2p \ ^3P_1\rangle.$$
(6)

The reduced matrix elements of the electric dipole operator for these basis states can all be written in terms of the one-electron line strength $S_{\rm H}$ for the transition 2s–2p:

$$\langle 2s^{2} {}^{1}S_{0} || \boldsymbol{d} || 2s2p {}^{1}P_{1} \rangle = \sqrt{2} \langle 2s || \boldsymbol{d} || 2p \rangle$$

$$\tag{7}$$

$$\langle 2p^{2} {}^{1}S_{0}||d||2s2p {}^{1}P_{1}\rangle = \sqrt{\frac{2}{3}}\langle 2p||d||2s\rangle = -\sqrt{\frac{2}{3}}\langle 2s||d||2p\rangle$$
(8)

$$\langle 2l^{2-1}S_0 || d || 2s2p^{-3}P_1 \rangle = 0$$
(9)

with

$$S_{\rm H} = |\langle 2\mathbf{s} || \mathbf{d} || 2\mathbf{p} \rangle|^2 \,. \tag{10}$$

The minus sign in equation (8) is important as it leads to destructive interference in these transition amplitudes at high Z:

$$S(\text{Res}) \equiv |\langle \Psi_0 || \boldsymbol{d} || \Psi_1 \rangle|^2 = \frac{2}{3} \cos^2 \theta \ (\sqrt{3} \cos \phi - \sin \phi)^2 S_{\text{H}}$$
(11)

$$S(\text{Int}) \equiv |\langle \Psi_0 || d || \Psi_3 \rangle|^2 = \frac{2}{3} \sin^2 \theta \, (\sqrt{3} \cos \phi - \sin \phi)^2 S_{\text{H}} \,. \tag{12}$$

Two observations can be made. The first is that these approximations suggest that the two line strengths have the ratio $S(\text{Int})/S(\text{Res}) = \tan^2\theta$. Thus they can be made commensurate by defining effective mixing-reduced line strengths $S_r(\text{Res})$ and $S_r(\text{Int})$ as

$$S_{\rm r}({\rm Res}) \equiv S({\rm Res})/\cos^2\theta$$
 (13)

$$S_{\rm r}({\rm Int}) \equiv S({\rm Int}) / \sin^2 \theta \,. \tag{14}$$

The second observation is that at high Z both matrix elements will approach the hydrogenlike limit

$$S_{\rm r}({\rm Res}) \cong S_{\rm r}({\rm Int}) \Rightarrow \frac{2}{3}(\sqrt{3}\cos\phi - \sin\phi)^2 S_{\rm H}/Z^2$$
. (15)

Thus a systematization of the data can be achieved by determining the singlet–triplet mixing angle θ from energy level data for each member of the sequence, and by theoretically calculating the non-relativistic high-Z limit of the 2s²–2p² mixing angle ϕ .

A formalism for the specification of θ has already been developed. For a pure *nsn*p configuration in intermediate coupling, θ can be specified from the splittings among the four energy levels. Since three energy intervals are specified by only two Slater parameters (the exchange and spin–orbit energies), θ is overdetermined, and can be specified in alternative ways that may not precisely agree if configuration interaction is present. If the measured excitation energies of the levels are designated by their limiting *LS* coupling symbols ³P₀, ³P₁, ³P₂ and ¹P₁, one way of prescribing the mixing angle has been suggested [5]

$$\cot(2\theta) = \pm \frac{1}{\sqrt{2}} \left[\frac{3({}^{3}P_{1} + {}^{1}P_{1} - 2{}^{3}P_{1})}{2({}^{3}P_{2} - {}^{3}P_{0})} - 1 \right].$$
(16)

If configuration interaction were present, other reductions for θ (e.g. using only two of the three energy intervals) would be expected to disagree slightly from that of equation (16). Disagreements between alternative reductions of θ thus provide a test of the presence of intermediate coupling. The Landé interval rule, generalized to include intermediate coupling

$$\frac{{}^{3}P_{2} - {}^{3}P_{1}}{{}^{3}P_{1} - {}^{3}P_{0}} = \frac{2 + \sqrt{2}\tan\theta}{1 - \sqrt{2}\tan\theta}$$
(17)

conveniently provides such a test. The Landé ratio can be formed from the observed triplet data alone, and compared with the results predicted for this ratio by θ as obtained from all four levels using equation (16). If this equality is satisfied to within experimental uncertainties, it indicates that configuration interaction is either slight, or is taken into account through the effective values of the mixing angle.

The high-Z limiting value of the $2s^2-2p^2$ mixing was computed by diagonalizing the 2 × 2 matrix of the Coulomb repulsion using standard Slater-integral methods, with unscreened hydrogenic radial wavefunctions, and the symbolic algebra package Maple [11], with the result $\phi = 0.227$ rad (13°). Combining this with the n = 2, J = 1 value $S_{\rm H} = 27$ obtained from equation (2) predicts the high-Z asymptote $S'_{\rm H}$

$$S'_{\rm H} \equiv \frac{2}{3} (\sqrt{3} \cos \phi - \sin \phi)^2 S_{\rm H} = 38.5 \,. \tag{18}$$

The linearizing exposition consists of reducing the measured and theoretically computed lifetime data to values for $S_r(\text{Res})$ and $S_r(\text{Int})$, examining them for the isoelectronic behaviour given in equation (1), and comparing the high-Z trend with the value for S'_H given in equation (18). Thus one of the goals of this study was to determine the degree to which the trend of empirical data displayed in this exposition approaches the value 38.5 in the high-Z limit.

3. Results

Transition wavelengths and empirical singlet-triplet mixing angles were deduced from observed spectroscopic data sources [12–19] for $4 \le Z \le 36$, wavelengths were taken from [19] for $37 \le Z \le 42$, and the results were extrapolated to Z = 54 using available theoretical calculations [20]. The degree to which the single configuration model of the mixing angle is valid was checked by computing the Landé interval from both the observed data and the mixing angle, according to equation (16). The results are shown in figure 1, and demonstrate that for $6 \le Z \le 54$ configuration interaction is either small, or else its inclusion in the effective value of θ correctly describes its effect on the energy level data. For Be I and B II

the effects of configuration interaction become significant both because the singlet-triplet mixing is itself small and because the central potential is less dominant. Since $\cos \theta$ is much less sensitive than $\sin \theta$ to discrepancies at small θ , the mixing angle formulation describes the resonance transition much better than the intercombination transition near the neutral end of the sequence. Thus no lifetime predictions for the intercombination transitions in Be I or B II were made. Although one cannot rigourously preclude the existence of configuration interaction effects that perturb the line strengths but not the energy levels, figure 1 clearly indicates that the mixing angle formulation is very effective in describing this system.



Figure 1. Plot of the Landé ratio $({}^{3}P_{2} - {}^{3}P_{1})/({}^{3}P_{1} - {}^{3}P_{0})$ obtained: +, directly from the observed levels; and \bigcirc , through the single configuration model using equations (16) and (17).

In order to verify and extend the study made in [5], all available measured lifetime data and quoted uncertainties for the resonance [21–60] and intercombination [61–66] transitions were assembled and are listed in table 1. A weighted least-squares fit was attempted which included all 47 data points in the resonance transition database. This yielded a value $\chi^2 = 123$ with 44 degrees of freedom, corresponding to an unacceptably low χ^2 probability. It can be seen from table 1 that this data base contains discrepancies that cannot be resolved by the quoted uncertainties, and it was necessary to perform a critical evaluation that rejects less reliable measurements on other grounds. To avoid biasing the fit, we performed this evaluation in two steps, first selecting data for inclusion on the basis of the analysis techniques used in the measurements, and then excluding data that exhibit severe deviations from isoelectronic trends. The values selected can be identified by the listing in table 1 of the corresponding value for Z^2S_r .

In the evaluation of the resonance transition data, we favoured results that accounted for cascade repopulation through the use of the ANDC method [67], or that in other ways sought to provide realistic and small uncertainties. An exception occurred for Al x, where a measurement [52] that reportedly used ANDC methods yielded a lifetime that was significantly longer than that indicated by the isoelectronic trend. Generally the more recent measurements were selected, particularly when earlier measurements disagreed and had unrealistically small quoted uncertainties. Both of the available measurements for Cl XIV were well off the isoelectronic trend and were rejected. In the case of the intercombination transition data, the only measurements available for low Z are for C III [61, 62], and concerns

| | | Reso | nance | Intercombination | | | |
|----|-----|---|---|------------------|--|--|----------------|
| Ζ | Ion | τ Obs.(Unc.) | [Ref.] | $Z^2 S_r$ | τ Obs.(Unc.) | [Ref.] | $Z^2 S_r$ |
| 4 | Be | $\begin{array}{c} 2.3(1)\times 10^{-9}\\ 2.05(6)\times 10^{-9}\\ 1.80(15)\times 10^{-9}\\ 1.85(7)\times 10^{-9} \end{array}$ | [21] ^a [22] ^a [23] ^a [24] | 166(6) | | | |
| 5 | В | $\begin{array}{l} 9.0(20)\times 10^{-10}\\ 1.15(10)\times 10^{-9}\\ 9.9(5)\times 10^{-10}\\ 1.17(7)\times 10^{-9}\\ 8.6(7)\times 10^{-10} \end{array}$ | [25] ^a [26] ^a [27] ^a [28] ^a [29] ^b | 109(9) | | | |
| 6 | С | $\begin{array}{l} 6.6(3) \times 10^{-10} \\ 6.4(6) \times 10^{-10} \\ 6.6(7) \times 10^{-10} \\ 5.0(3) \times 10^{-10} \\ 5.7(2) \times 10^{-10} \end{array}$ | [30] ^a [31] ^a [32] ^a [33] ^a [34] ^b | 87(3) | $\begin{array}{l} 1.3(4)\times 10^{-2}\\ 8.3(5)\times 10^{-3}\\ 9.6(4)\times 10^{-3}\\ 9.7(3)\times 10^{-3} \end{array}$ | [61] ^a [62] ^a [72] ^c [73] ^c | 68(3) 67(2) |
| 7 | Ν | $\begin{array}{l} 5.3(8) \times 10^{-10} \\ 5.3(8) \times 10^{-10} \\ 4.39(22) \times 10^{-10} \\ 4.6(9) \times 10^{-10} \\ 5.0(3) \times 10^{-10} \\ 4.25(15) \times 10^{-10} \\ 5.0(7) \times 10^{-10} \end{array}$ | [35] ^a [36] ^a [37] ^a [38] ^a [33] ^a [39] ^b [40] ^a | 76(3) | 1.72(3)×10 ⁻³ | [74] ^c | 58(1) |
| 8 | 0 | $\begin{array}{l} 4.3(5)\times 10^{-10}\\ 4.12(17)\times 10^{-10}\\ 3.8(2)\times 10^{-10}\\ 4.9(5)\times 10^{-10}\\ 3.6(4)\times 10^{-10}\\ 3.38(15)\times 10^{-10} \end{array}$ | $\begin{array}{c} [41]^{a} \\ [42]^{a} \\ [43]^{a} \\ [44]^{a} \\ [45]^{a} \\ [39]^{b} \end{array}$ | 70(3) | | | |
| 9 | F | $\begin{array}{l} 3.7(2)\times 10^{-10}\\ 3.1(4)\times 10^{-10} \end{array}$ | [46] ^a [47] | 59(8) | | | |
| 10 | Ne | $\begin{array}{l} 2.9(2)\times10^{-10}\\ 2.41(25)\times10^{-10}\\ 2.32(37)\times10^{-10}\end{array}$ | [48] ^a [42] ^a [49] | 64(10) | | | |
| 12 | Mg | $1.90(15) \times 10^{-10}$ | [50] | 56(4) | | | |
| 13 | Al | $\begin{array}{l} 1.75(15)\times 10^{-10}\\ 1.9(3)\times 10^{-10}\\ 1.92(15)\times 10^{-10} \end{array}$ | [50] [51] ^a [52] ^{a, b} | 53(5) | | | |
| 14 | Si | $\begin{array}{l} 1.55(10)\times10^{-10}\\ 1.8(1)\times10^{-10}\\ 1.50(12)\times10^{-10}\end{array}$ | [53] ^a [54] ^a [50] | 54(4) | | | |
| 15 | Р | $\begin{array}{l} 1.45(10)\times 10^{-10}\\ 1.40(10)\times 10^{-10} \end{array}$ | [55] ^a [50] | 51(4) | | | |
| 16 | S | $1.57(16) \times 10^{-10}$ $1.30(15) \times 10^{-10}$ | [56] ^a [50] | 49(6) | | | |
| 17 | Cl | $\begin{array}{l} 1.5(3) \times 10^{-10} \\ 1.4(1) \times 10x^{-10} \end{array}$ | [57] ^a [58] ^a | | | | |
| 26 | Fe | $5.1(5) \times 10^{-11}$ | [59] | 47(5) | $1.3(4) \times 10^{-8}$ | [63] ^a | |
| 36 | Kr | $1.75(15) \times 10^{-11}$ | [60] | 47(4) | $\begin{array}{l} 2.3(3)\times 10^{-9} \\ 2.54(24)\times 10^{-9} \end{array}$ | [64] [65] ^a | 39(5) |
| 54 | Xe | | | | $4.7(5) \times 10^{-10}$ | [66] | 36(4) |

Table 1. Database for Be-like $2s2p^{1,3}P_1$ lifetimes (in seconds). The value for Z^2S_r is listed for the entries critically selected for inclusion in the plot and fits.

^a Excluded from plot.
 ^b ANDC cascade analysis.
 ^c Precise theoretical calculation.

| | Resonance τ (s) | | | Intercombination τ (s) | | | |
|----|----------------------|------------------------|----------------------------|-----------------------------|------------------------|--------------------------|---------------|
| Ζ | λ (Å) | Pred. | Obs. ^a | λ (Å) | Pred. | Obs. ^a | $\sin \theta$ |
| 4 | 2349.3 | 1.850×10^{-9} | $1.85(7) \times 10^{-9}$ | 4549.9 | | | 0.000 069 |
| 5 | 1362.5 | 8.61×10^{-10} | $8.6(7) \times 10^{-10}$ | 2677.9 | _ | | 0.000 282 |
| 6 | 977.0 | $5.69 	imes 10^{-10}$ | $5.7(2) \times 10^{-10}$ | 1908.7 | 9.77×10^{-3} | $9.7(3) \times 10^{-3}$ | 0.000755 |
| 7 | 765.1 | 4.27×10^{-10} | $4.25(15) \times 10^{-10}$ | 1486.5 | 1.71×10^{-3} | $1.72(3) \times 10^{-3}$ | 0.001 539 |
| 8 | 629.7 | 3.42×10^{-10} | $3.38(15) \times 10^{-10}$ | 1218.4 | 4.29×10^{-4} | | 0.002723 |
| 9 | 535.2 | 2.85×10^{-10} | $3.1(4) \times 10^{-10}$ | 1032.5 | 1.36×10^{-4} | | 0.004 382 |
| 10 | 465.2 | 2.44×10^{-10} | $2.32(37) \times 10^{-10}$ | 895.2 | 5.01×10^{-5} | | 0.006 624 |
| 11 | 411.2 | 2.13×10^{-10} | | 789.8 | 2.12×10^{-5} | | 0.00947 |
| 12 | 368.1 | 1.88×10^{-10} | $1.9(15) \times 10^{-10}$ | 706.0 | 9.84×10^{-6} | | 0.013 00 |
| 13 | 332.8 | $1.68 	imes 10^{-10}$ | $1.92(15) \times 10^{-10}$ | 637.8 | 4.91×10^{-6} | | 0.017 35 |
| 14 | 303.3 | 1.51×10^{-10} | $1.50(12) \times 10^{-10}$ | 580.9 | 2.62×10^{-6} | | 0.02248 |
| 15 | 278.3 | 1.37×10^{-10} | $1.40(10) \times 10^{-10}$ | 532.8 | 1.46×10^{-6} | | 0.028 56 |
| 16 | 256.7 | 1.25×10^{-10} | $1.30(15) \times 10^{-10}$ | 491.5 | 8.53×10^{-7} | | 0.035 59 |
| 17 | 237.8 | 1.14×10^{-10} | $1.4(1) \times 10^{-10}$ | 455.5 | $5.18 	imes 10^{-7}$ | | 0.043 60 |
| 18 | 221.1 | 1.04×10^{-10} | | 424.0 | 3.27×10^{-7} | | 0.05249 |
| 19 | 206.2 | 9.53×10^{-11} | | 396.0 | 2.13×10^{-7} | | 0.06231 |
| 20 | 192.9 | $8.74 	imes 10^{-11}$ | | 371.0 | 1.41×10^{-7} | | 0.073 58 |
| 21 | 180.7 | 8.02×10^{-11} | | 348.6 | $9.58 	imes 10^{-8}$ | | 0.085 55 |
| 22 | 169.6 | 7.36×10^{-11} | | 328.3 | 6.69×10^{-8} | | 0.09843 |
| 23 | 159.3 | 6.75×10^{-11} | | 309.9 | 4.75×10^{-8} | | 0.1124 |
| 24 | 149.9 | 6.18×10^{-11} | | 293.2 | 3.43×10^{-8} | | 0.1273 |
| 25 | 141.1 | 5.66×10^{-11} | | 277.8 | 2.54×10^{-8} | | 0.1427 |
| 26 | 132.9 | 5.17×10^{-11} | $5.1(5) \times 10^{-11}$ | 263.8 | 1.90×10^{-8} | | 0.1591 |
| 27 | 125.2 | 4.71×10^{-11} | | 250.8 | $1.46 	imes 10^{-8}$ | | 0.1755 |
| 28 | 118.0 | 4.30×10^{-11} | | 238.8 | 1.13×10^{-8} | | 0.1924 |
| 29 | 111.2 | $4.90 	imes 10^{-11}$ | | 227.8 | $8.88 	imes 10^{-9}$ | | 0.2098 |
| 30 | 104.7 | 3.53×10^{-11} | | 217.7 | 7.12×10^{-9} | | 0.2268 |
| 31 | 98.58 | 3.19×10^{-11} | | 208.2 | 5.77×10^{-9} | | 0.2440 |
| 32 | 92.90 | 2.88×10^{-11} | | 199.4 | 4.72×10^{-9} | | 0.2613 |
| 33 | 87.35 | 2.58×10^{-11} | | 191.3 | 3.94×10^{-9} | | 0.2777 |
| 34 | 82.29 | 2.32×10^{-11} | | 183.6 | 3.30×10^{-9} | | 0.2943 |
| 35 | 77.28 | 2.07×10^{-11} | | 176.7 | 2.83×10^{-9} | | 0.3096 |
| 36 | 72.76 | $1.85 	imes 10^{-11}$ | $1.75(15) \times 10^{-11}$ | 169.8 | 2.42×10^{-9} | $2.3(3) \times 10^{-9}$ | 0.3252 |
| 37 | 68.38 | 1.64×10^{-11} | | 163.6 | 2.10×10^{-9} | | 0.3392 |
| 38 | 64.25 | 1.45×10^{-11} | | 157.8 | 1.85×10^{-9} | | 0.3518 |
| 39 | 60.34 | 1.27×10^{-11} | | 152.3 | 1.65×10^{-9} | | 0.3636 |
| 40 | 56.65 | 1.12×10^{-11} | | 147.2 | 1.47×10^{-9} | | 0.3754 |
| 41 | 53.18 | $9.89 	imes 10^{-12}$ | | 142.4 | $1.31 	imes 10^{-9}$ | | 0.3877 |
| 42 | 49.90 | 8.80×10^{-12} | | 137.8 | 1.17×10^{-9} | | 0.4007 |
| 43 | 46.91 | 7.77×10^{-12} | | 133.4 | $1.06 	imes 10^{-9}$ | | 0.4122 |
| 44 | 44.04 | 6.81×10^{-12} | | 129.4 | 9.61×10^{-10} | | 0.4222 |
| 45 | 41.29 | 5.94×10^{-12} | | 125.5 | $8.83 	imes 10^{-10}$ | | 0.4309 |
| 46 | 38.70 | $5.16 	imes 10^{-12}$ | | 121.9 | $8.16 	imes 10^{-10}$ | | 0.4389 |
| 47 | 36.26 | 4.48×10^{-12} | | 118.4 | 7.56×10^{-10} | | 0.4463 |
| 48 | 33.98 | 3.88×10^{-12} | | 115.0 | 7.01×10^{-10} | | 0.4537 |
| 49 | 31.87 | 3.37×10^{-12} | | 111.8 | 6.51×10^{-10} | | 0.4608 |
| 50 | 29.91 | 2.93×10^{-12} | | 108.6 | $6.05 	imes 10^{-10}$ | | 0.4673 |
| 51 | 28.09 | 2.55×10^{-12} | | 105.6 | $5.64 	imes 10^{-10}$ | | 0.473 5 |
| 52 | 26.38 | 2.21×10^{-12} | | 102.8 | $4.29 	imes 10^{-10}$ | | 0.4793 |
| 53 | 24.78 | 1.92×10^{-12} | | 100.3 | $5.00 	imes 10^{-10}$ | | 0.4850 |
| 54 | 23.27 | 1.67×10^{-12} | | 98.1 | 4.74×10^{-10} | $4.7(5) \times 10^{-10}$ | 0.4905 |
| | | | | | | | |

Table 2. Lifetime predictions (in seconds) obtained by fitting equation (1) to measured data.

^a Observed values as critically selected in table 1.

have been raised [72, 73] that both of these measurements lie outside theoretical error bounds. Since highly precise calculations for C III [72, 73] and for N IV [74] (which include error bounds) have recently been made, we have here utilized these theoretical values in place of experimental measurements. For Fe XXIII the measured value was far off the isoelectronic trend and was rejected. With this critical evaluation, the database differs from that used in [5] for Z = 9 and 36 for the resonance transitions and Z = 6, 7 and 26 for the intercombination line.

These values are displayed plotted against the reciprocal screened charge in figure 2. The trend of the experimental points is compared with recent precise theoretical calculations ([70] for the resonance transitions and [71] for the intercombination transitions). It is clear that the high-*Z* trend of both the data and the calculations is consistent with the non-relativistic asymptotic value $S'_{\rm H} = 38.5$.



Figure 2. Plot of the charge-scaled reduced line strength versus the reciprocal screened charge. The symbols denote measured values for the resonance (\times) and intercombination (\bigcirc) transitions. The curves trace theoretical calculations for the resonance (—) and intercombination (- - -) transitions. The non-relativistic $1/Z \Rightarrow 0$ limit is indicated by (\blacklozenge).

A linear fit was performed to both sets of data. The fits yielded $S_{\rm H} = 40.01$, B = 151.9, C = 2.8, with $\chi^2 = 1.6$ (14 data points and three fitting parameters) for the resonance transition data, and $S_{\rm H} = 33.66$, B = 105.3 (using the same value of *C*), with $\chi^2 = 0.49$ (five data points and two fitting parameters) for the intercombination line. These fits were used to produce the smoothed and interpolated values for $4 \le Z \le 54$ that are given in table 2, together with the transition wavelengths and the singlet–triplet mixing angles. This critical compilation and fitting confirms the values for the resonance transition reported in [5], and corrects values for low-*Z* members for the intercombination transition reported in [5] that were affected by the use of a crucial but imprecise measurement for C III [61].

The accuracy of these predictions is dependent not only on the precision of the fit, but also on the validity of the linearity expressed in equation (1), the correctness of the quoted uncertainties in the database, and the judgement we have exercised in making our critical selection within the database. At the neutral end of the sequence it is clear that *ab initio*

theoretical methods can provide accuracies within 1% or better (e.g. the calculations of Weiss [68] for Be I and B II and of Godefroid *et al* [69] for B II), and that higher order terms in 1/(Z - C) could distort the linearity of equation (1) at low Z. Similarly, at very high Z relativistic mixing could distort the value of the non-relativistic limit $Z^2S_r = 38.5$. However, in the range $26 \le Z \le 54$, the linear empirical trends in this exposition appear to offer predictive capabilities of within 10% or better, which could be improved as more precise measurements become available.

4. Conclusions

The utilitarian value of this systematization in critically evaluating, smoothing, and extrapolating line strength data for this system is manifested by the degree to which the mixing angle reduction reproduces the overdetermined energy intervals in figure 1 and by the nearly linear regularity of the reduced line strength exposition in figure 2. Moreover, the clear tendency for both the experimental and theoretical data to approach the asymptotic configuration-mixed hydrogen limit at high *Z* suggests that a few very precise measurements at lower *Z* could be extrapolated to relatively high *Z* with predictive accuracy. Since these high-*Z* lifetimes are too short for time-of-flight methods and too long for linewidth studies, empirical extrapolations are valuable. For very high *Z*, relativistic effects must be considered. A procedure for including relativistic corrections to the hydrogen-like calculation has already been applied [4] to the alkali-like sequences. At very high *Z* similar corrections must also be made here, as well as an evaluation of the relativistic limit of the ground-state configuration mixing. The linearity of this systematization can be further tested and the accuracy of its predictions can be refined as additional measurements become available.

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References

- [1] Edlén B 1979 Phys. Scr. 17 565
- [2] Reistad N and Martinson I 1986 Phys. Rev. A 54 2632
- [3] Träbert E 1988 Z. Phys. D 9 143
- [4] Curtis L J, Ellis D G and Martinson I 1995 Phys. Rev. A 51 251
- [5] Curtis L J 1991 Phys. Scr. 43 137
- [6] Curtis L J 1992 J. Opt. Soc. Am. B 9 5
- [7] Träbert E and Curtis L J 1993 Phys. Scr. 48 586
- [8] Curtis L J 1993 J. Phys. B: At. Mol. Opt. Phys. 26 L589
- [9] Curtis L J 1992 J. Phys. B: At. Mol. Opt. Phys. 25 1427
- [10] Curtis L J et al 1995 Phys. Rev. A 51 4575
- [11] Maple Reference Manual (Waterloo, Ontario: WATCOM)
- [12] Johansson L 1962 Ark. Fys. 23 119
- [13] Ölme A 1970 Phys. Scr. 1 256
- [14] Bockasten K 1955 Ark. Fys. 9 457
- [15] Hallin R 1966 Ark. Fys. 32 201
- [16] Bockasten K and Johansson K B 1968 Ark. Fys. 38 563
- [17] Engström L 1985 Phys. Scr. 31 379
- [18] Edlén B 1983 Phys. Scr. 28 51

- [19] Denne B, Magyar G and Jacquinot J 1989 Phys. Rev. A 40 3702
- [20] Cheng K-T, Kim Y-K and Desclaux J P 1979 At. Data Nucl. Data Tables 24 11
- [21] Andersen T, Jessen K A and Sørensen G 1969 Phys. Rev. 188 7681
- [22] Bergström I, Bromander J, Buchta R, Lundin L and Martinson I 1969 Phys. Lett. 28A 721
- [23] Hontzeas S, Martinson I, Erman P and Buchta R 1974 Phys. Scr. 6 55
- [24] Martinson I, Gaupp A and Curtis L J 1974 J. Phys. B: At. Mol. Phys. 7 L463
- [25] Lawrence G and Savage B D 1966 Phys. Rev. 141 67
- [26] Martinson I, Bickel W S and Ölme A 1970 J. Opt. Soc. Am. 60 1213
- [27] Bromander J 1971 Phys. Scr. 4 61
- [28] Kernahan J A, Pinnington E H, Livingston A E and Irwin D J G 1975 Phys. Scr. 12 319
- [29] Bashkin S, McIntyre L C, v Buttlar H, Ekberg J O and Martinson I 1985 Nucl. Instrum Methods B 9 593
- [30] Heroux L 1969 Phys. Rev. 180 1
- [31] Poulizac M C and Buchet J P 1971 Phys. Scr. 4 191
- [32] Buchet-Poulizac M C and Buchet J P 1973 Phys. Scr. 8 40
- [33] Chang M W 1977 Astrophys. J. 211 300
- [34] Reistad N, Hutton R, Nilsson A E, Martinson I and Mannervik S 1986 Phys. Scr. 34 151
- [35] Berry H G, Bickel W S, Bashkin S, Désesquelles J and Schectman R M 1971 J. Opt. Soc. Am. 61 947
- [36] Buchet J P, Poulizac M C and Carre M 1972 J. Opt. Soc. Am. 62 623
- [37] Kernahan J A, Livingston A E and Pinnington E H 1974 Can. J. Phys. 52 1895
- [38] Dumont P D, Biémont E and Grevesse N 1974 J. Quant. Spectrosc. Radiat. Transfer 14 1127
- [39] Engström L, Denne B, Ekberg J O, Jones K W, Jupén C, Litzén U, Meng W T, Trigueiros A and Martinson I 1981 Phys. Scr. 24 551
- [40] Ishii K, Suzuki, M and Takahashi, J 1985 J. Phys. Japan 54 3742
- [41] Martinson I, Berry H G, Bickel W S and Oona H 1971 J. Opt. Soc. Am. 61 519
- [42] Irwin D J G, Livingston A E and Kernahan J A 1973 Nucl. Instrum. Methods 110 105
- [43] Pinnington E H, Irwin D J G, Livingston A E and Kernahan J A 1974 Can. J. Phys. 52 1961
- [44] Knystautas E J and Drouin R 1975 J. Phys. B: At. Mol. Phys. 8 2001
- [45] Buchet J P, Buchet-Poulizac M C and Druetta M 1976 J. Opt. Soc. Am. 66 842
- [46] Barrette L and Drouin R 1973 Can. J. Spectrosc. 18 50
- [47] Knystautas E J, Buchet-Poulizac M C, Buchet J P and Druetta M 1979 J. Opt. Soc. Am. 69 474
- [48] Beauchemin G, Kernahan J A, Irwin D G J and Drouin R 1972 Phys. Lett. 40A 194
- [49] Irwin D J G, Livingston A E and Kernahan J A 1973 Can. J. Phys. 51 1948
- [50] Träbert E and Heckmann P H 1980 Phys. Scr. 22 489
- [51] Druetta M, Jacques C and Knystautas E J 1983 J. Phys. B: At. Mol. Phys. 16 167
- [52] Ando K, Kohmoto S, Awaya Y, Kumagai H, Tonuma T and Tsurubuchi S 1988 Nucl. Instrum Methods B 33 239
- [53] Träbert E, Heckmann P H and v Buttlar H 1977 Z. Phys. A 281 333
- [54] Pegg D J, Griffin P M, Alton G D, Elston S B, Forester J P, Suter M, Thoe R S and Vane C R 1978 Phys. Scr. 18 18
- [55] Träbert E and Heckmann P H 1981 Phys. Scr. 21 35
- [56] Pegg D J, Forester J P, Vane C R, Elston S B, Griffin P M, Groeneveld K-O, Peterson R S, Thoe R S and Sellin I A 1977 Phys. Rev. A 15 1958
- [57] Forester J P, Pegg D J, Griffin P M, Alton G D, Elston S B, Hayden H C, Thoe R S, Vane C R and Wright J J 1978 Phys. Rev. A 18 1476
- [58] Kawatsura K, Sataka M, Ootuka A, Komaki K, Naramoto H, Ozawa K, Nakai Y and Fujimoto F 1987 Nucl. Instrum. Methods A 262 150
- [59] Buchet J P, Buchet-Poulizac M C, Denis A, Désesquelles J, Druetta M, Grandin J P, Huet M, Husson X and Lecler D 1984 Phys. Rev. A 30 309
- [60] Träbert E, Doerfert J, Granzow J, Büttner R, Brauckhoff J, Nicolai M, Schartner K-H, Folkmann F and Mokler P H 1995 Phys. Lett. 202A 91
- [61] Smith P L, Johnson B C, Kwong H S and Parkinson W H 1984 Phys. Scr. T 8 88
- [62] Kwong V H S, Fang Z, Gibbons T T, Parkinson W H and Smith P L 1993 Astrophys. J. 411 431
- [63] Dietrich D D, Leavitt J A, Bashkin S, Conway J G, Gould H, MacDonald D, Marrus R, Johnson B M and Pegg D J 1978 Phys. Rev. A 18 208
- [64] Dietrich D D, Leavitt J A, Gould H and Marrus R 1980 Phys. Rev. A 22 1109 Dietrich D D and Leavitt J A 1979 J. Physique (Colloque C1) 40 217
- [65] Livingston A E, Kukla K W, Vogel Vogt C M, Berry H G, Dunford R W, Curtis L J and Cheng S 1995 Bull. Am. Phys. Soc. 40 1324

- [66] Möller G, Träbert E, Lodwig V, Wagner C, Heckmann P H, Blanke J H, Livingston A E and Mokler P H 1989 Z. Phys. D 11 333
- [67] Curtis L J, Berry H G and Bromander J 1971 Phys. Lett. 34A 169
- [68] Weiss A W 1995 Phys. Rev. A 51 1067
- [69] Godefroid M, Olsen J, Jönsson P and Froese Fischer C 1995 Astrophys. J. 450 473
- [70] Fleming J, Vaeck N, Hibbert A and Godefroid M R 1995 Phys. Scr. at press
- [71] Ynnerman A and Froese Fischer C 1995 Phys. Rev. A 51 2020
- [72] Fleming J, Hibbert A and Stafford R P 1994 Phys. Scr. 49 316
- [73] Froese Fischer C 1994 Phys. Scr. 49 323
- [74] Fleming J, Brage T, Bell K L, Vaeck N, Hibbert A, Godefroid M and Froese Fischer C 1995 Astrophys. J. at press