

Table 8. Scaling

Sequence	B_α	d_α	p_α	B_β	d_β	p_β
Mg	2427	2.43	3.18	1148	0.61	3.37
Zn	504.7	1.96	2.42	2545	1.74	3.40
Cd	548.0	2.04	2.38	2667	1.78	3.28
Hg	231.4	2.05	2.08	1509	2.09	3.15

so the ratio of the bracketing width to the lower limit of β decreases even faster, as $1/\zeta^2$. For α_d the relationship is more complicated, but for very large Z the bracketing and the upper limit scale together.

6.3. Charge scaling of the results

The polarizability data in tables 4 - 7 were fitted to the charge scaling equations

$$\alpha_d = \frac{B_\alpha}{(\zeta + d_\alpha)^{p_\alpha}} ; \quad \beta = \frac{B_\beta}{(\zeta + d_\beta)^{p_\beta}} . \quad (33)$$

The fitted values are listed in table 8.

7. Relativistic effects in the Hg sequence

Homologous comparisons of these four isoelectronic sequences reveal interesting trends. It can be seen from tables 4-7 that the oscillator strengths $f_{ns,np}$ decrease with increasing ionicity, consistent with the $\Delta n = 0$ scaling with $1/\zeta$ that was predicted in equation (30). However, table 7 reveals that for the Hg sequence the oscillator $f_{6s,6p}$ is nearly constant over the sequence, as would be expected for a $\Delta n \neq 0$ transition as predicted in equation (29). In all four sequences the $E_{ns,np}$ energy decreases with ζ as expected, so the difference in scaling resides in the line strength factor.

The origin of this behavior lies in significant relativistic corrections that affect Hg and its isoelectronic sequence [76, 77]. In earlier studies of the Cd [45] and Hg [31] sequences, multiconfiguration Dirac Hartree Fock (MCDHF) calculations showed that $6s^2$ and $6s6p$ remain lower than plunging levels from the $5f$ and $5g$ subshells for all ions through uranium. In contrast, for the Cd sequence, plunging levels from the $4f$ subshell perturb the $5s5p$ levels above $Z=60$ and for $Z > 62$ the $4f$ levels replace $5s^2$ as the ground state. Moreover, whereas the mixing angle reduction could be accomplished using the Schrödinger formalism with LS coupling for the Mg, Zn, and Cd sequences, MCDHF calculations for the Hg sequence indicated a significant difference between the Dirac transition matrices $\langle s_{1/2}|r|p_{1/2} \rangle$ and $\langle s_{1/2}|r|p_{3/2} \rangle$, requiring use of the Dirac formalism and jj coupling.

The reasons for these observations are closely related to the unusual fact that mercury is a liquid at ambient temperatures. The $6s$ electron (and each s electron in the core) is drawn in because of relativistic effects at small r . It can be made plausible in terms of the Bohr orbit picture, since the speed of the $6s$ electron at periapsis is $v \approx Zc/137$ (for $Z=80$, $v = 0.58c$). The increase in the relativistic mass causes the effective Bohr radius to shrink (although Zitterbewegung and the Darwin term decrease the effect somewhat). Moreover, the magnetic coupling of the two

paired s electrons is enhanced by the predominance of jj coupling, since spin-own-orbit coupling to the nucleus dominates over spin-spin, orbit-orbit and spin-other-orbit coupling to other electrons. Thus mercury atoms and ions in the Hg sequence behave more like an inert gas than an alkaline earth.

It has been noted [76] that gold and mercury differ in melting points, densities, electrical conductivities, the ability to amalgamate with noble metals, *etc.*, by greater factors than virtually any other pair of neighbors in the Periodic table. Similarly, Tl II is more stable than Tl I, Pb III is more stable than Pb II, and Bi IV is more stable than Bi III. Relativistic calculations have also explained the difference in color between gold and silver [77].

Only the first four members of the Hg sequence are radioactively stable, and measurements of the atomic structure properties of its radioactive members are lacking. However, the atomic properties of the radioactive members have applications in, *e.g.*, modeling calculations of radiation transfer in astrophysical and controlled fusion. Thus semiempirical extrapolations can provide useful estimates for the ions in this sequence with $Z \geq 84$.

8. Conclusions

For atomic systems in which the ground state oscillator strength is dominantly concentrated in one low-lying resonance transition, the method described here provides a powerful means to interconnect measurements and predictions of the quantities α_d , β , and τ . If a precision measurement of τ is available, α_d and β can be deduced. Alternatively, if a precision measurement of α_d is available, τ and β can be deduced. Moreover, screening parametrizations of line strength data permit isoelectronic interpolation of a few precise measurements to obtain estimates of these quantities for the entire sequence. The Mg, Zn, Cd and Hg sequences satisfy these criteria very well, and the results presented here provide an extensive data base spanning both homologous and isoelectronic sequences.

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References

- [1] B. Edlén B 1964 Atomic Spectra *Handb. der Physik XXVII* ed S Flügge (Berlin: Springer) pp 80-220, section 20
- [2] Dalgarno A and Kingston A E 1959 *Proc. Phys. Soc.* **74** 455-64
- [3] Curtis L J 2007 *J. Phys. B: At. Mol. Opt. Phys.* **40** 3173-80
- [4] Curtis L J, Berry H G and Bromander J 1971 *Phys. Lett.* **34A** 169-70
- [5] Curtis L J 2003 *Atomic Structure and Lifetimes: A Conceptual Approach* (Cambridge Univ. Press: Cambridge UK)
- [6] Kuhn W 1925 *Z. Physik* **33** 408-12
- [7] Reiche F and Thomas W 1925 *Z. Physik* **34** 510-25
- [8] Curtis L J 1991 *Can. J. Phys.* **69** 668-70
- [9] Miller T M and Bederson B 1977 *Adv. At. Mol. Phys.* **13**, 1-55
- [10] Kleinman C J, Hahn Y and Spruch L 1968 *Phys. Rev.* **165** 53-62

- [11] Johnson W R, Kolb D and Huang K-N 1983 *At. Data Nucl. Data Tables* **28** 333-40
- [12] Snow E and Lundein S R 2007 *Phys. Rev. A*, in press
- [13] Kuske P, Kirchner N, Wittman W, Andrä H J and Kaiser D 1978 *Phys. Lett. A* **64** 377
- [14] Andrä H J 1976 "Beam-Foil Spectroscopy, Vol. 2," eds. Sellin I A and Pegg D J (Plenum New York) p.835.
- [15] Guet C and Johnson W R 1991 *Phys. Rev. A* **44**, 1531-1535
- [16] Curtis L J 1989 *Phys. Rev. A* **40** 6958-68
- [17] Komara R A, Gearba M A, Fehrenbach C W and Lundein S R 2005 *J. Phys. B: At. Mol. Opt. Phys.* **38** S87-S95
- [18] NIST Physical Reference Data, <http://physics.nist.gov/PhysRefData/contents.html>
- [19] Tachiev G and Froese Fischer C 2002 "The MCHF/MCDHF Collection"
<http://atoms.vuse.vanderbilt.edu>
- [20] Berry H G, Bromander J, Curtis L J and Buchta R 1971 *Phys. Scr.* **3** 125-132
- [21] Livingston A E, Dumont P D, Baudinet-Robinet Y, Garnir H P, Biémont E and Grevesse N 1976 *Beam-Foil Spectroscopy*, eds I A Sellin and D J Pegg (Plenum, New York) 339-346
- [22] Safranova U, Johnson W R and Berry H G 2000 *Phys. Rev. A* **61**, 052503:1-11
- [23] Magnusson C E and Zetterberg P O 1977 *Phys. Scr.* **15** 237-250
- [24] Curtis L J, Martinson I and Buchta R 1971 *Phys. Scr.* **3** 197-202
- [25] Livingston A E, Kernahan J A, Irwin D J G and Pinnington E H 1975 *Phys. Scr.* **12** 223-229
- [26] Lundein S R and Fahrenbach C W 2007 *Phys. Rev. A* **75** 032523 1-7
- [27] Pinnington E H, Ansbacher W and Kernahan J A 1984 *J. Opt. Soc. Am. B* **1** 30-3
- [28] Liu L, Hutton R, Zou Y, Andersson M and Brage T 2006 *J. Phys. B: At. Mol. Opt. Phys.* **39** 3147-58
- [29] Chou H-S, Chi H-C and Huang K-N 1994 *Phys. Rev. A* **49** 2394-8
- [30] Ross C B, Wood D R and Scholl P S 1976 *J. Opt. Soc. Am.* **66** 36-9
- [31] Curtis L J, Irving R E, Henderson M, Matulioniene R, Froese Fischer C and Pinnington E. 2001 *Phys. Rev. A* **63** 042502:1-7
- [32] Haar R R, Beideck D J, Curtis L J, Kvale T J, Sen A, Schectman R M and Stevens H 1993 *Nuc. Instr. Meth. in Phys. Res.* **79** 746-8
- [33] Haar R R and Curtis L J 1994 *Nuc. Instr. Meth. in Phys. Res.* **79** 782-4
- [34] Provencher S W 1976 *J. Chem. Phys.* **64** 2772-7
- [35] Reistad N, Jupén C, Huldt S, Engström L and Martinson I 1985 *Phys. Scr.* **32** 164-8
- [36] Curtis L J 1971 "Proc. 2nd European Conf. on Beam Foil Spectroscopy" ed. M. Dufay, ed, Lyon France.
- [37] Hutton R, Reistad N, Martinson I, Träbert E, Heckmann P H, Blanke J H, Hellmann H M and Hucke R 1987 *Phys. Scr.* **35** 300-2
- [38] Engström L, Bengtsson P, Jupén C, Livingston A E and Martinson I 1995 *Phys. Rev. A* **51** 179-84
- [39] Reistad N, Engström L and Berry H G 1986 *Phys. Scr.* **34** 158-63
- [40] Träbert E, Pinnington E H, Kernahan J A, Doerfert J, Granzow J, Heckmann P H and Hutton R 1996 *J. Phys. B: At. Mol. Opt. Phys.* **29** 2647-59
- [41] Hutton R, Engström L and Träbert E 1988 *Nucl. Instr. Meth. in Phys. Res. B* **31** 294-9
- [42] Savitzky A and Golay M J E 1964 *Analytical Chemistry* **36** 1627-39
- [43] Curtis L J 1991 *Phys. Scr.* **43** 137-43
- [44] Curtis L 1992 *J. Opt. Soc. Am.* **9** 5-9
- [45] Curtis L J, Matulioniene R, Ellis D G and Froese Fischer C 2000 *Phys. Rev. A* **62** 052513:1-7
- [46] Curtis L J, Ellis D G and Martinson I 1995 *Phys. Rev. A* **51** 251-6
- [47] Liljeby L, Lindgård A, Mannervik S, Veje E and Jelenkovic B 1979 *Phys. Scr.* **21** 805
- [48] Kernahan, J A, Pinnington E H, O'Neill J A, Brooks R L and Donnelly K E 1979 *Phys. Scr.* **19** 267-70
- [49] Biémont E, Dumont P-D, Garnir H P, Palmeri P and Quinet P 2002 *Eur. J. Phys.* **20** 199-204
- [50] Martinson I, Curtis L J, Huldt S, Litzén U, Liljeby L, Mannervik S and Jelenkovic B 1979 *Phys. Scr.* **19** 17-21
- [51] Andersen T, Eriksen P, Poulsen O and Ramanujam P S 1979 *Phys. Rev. A* **20** 2621-4
- [52] Kaufman V and Sugar J 1987 *J. Opt. Soc. Am.* **4** 1919-23
- [53] Lurio A and Novick R 1964 *Phys. Rev.* **134** A608-14
- [54] Ansbacher W, Pinnington E H, Kernahan J A and Gosselin R N 1986 *Can. J. Phys.* **64** 1365-8
- [55] Pinnington E H, Kernahan J A and Ansbacher W 1987 *Can. J. Phys.* **65** 7-12
- [56] Pinnington E H, Ansbacher W, Kernahan J A, Gosselin R N, Bahr J L and Inamdar A S 1985 *J. Opt. Soc. Am. B* **2** 1653-7
- [57] Pinnington E H, Ansbacher W and Kernahan J A 1987 *J. Opt. Soc. Am. B* **4** 696-7

- [58] Pinnington E H, Ansbacher W, Kernahan J A and Inamdar A S 1985 *J. Opt. Soc. Am. B* **2** 331-5
- [59] Ansbacher W, Pinnington E H, Tauheed A and Kernahan J A 1991 *J. Phys. B: At. Mol. Opt. Phys.* **24** 587-93
- [60] O'Neill J A, Pinnington E H, Donnelly K E and Brooks R L 1979 *Phys. Scr.* **20** 60-4
- [61] Kernahan J A, Pinnington E H, O'Neill J A, Bahr J L and Donnelly K E 1980 *J. Opt. Soc. Am.* **70** 1126-30
- [62] Moore C E 1952 *Atomic Energy Levels, Vol. 3*, NSRDS-NBS 35 (Reissued Dec. 1971).
- [63] Andersen T and Sørensen G 1973 *J. Quant. Spectrosc. Radiative Transf.* **13** 369-76
- [64] Lurio A 1965 *Phys. Rev. A* **140** A1505-8
- [65] Skerbele A and Lassetre E N 1972 *J. Chem. Phys.* **52** 2708-11
- [66] Abjean R and Johannin-Gilles A 1976 *J. Quant. Spectrosc. Radiative Transf.* **16** 369-71
- [67] Pinnington E H, Ansbacher W, Kernahan J A, Ahmad T and Ge Z-Q 1988 *Can. J. Phys.* **66** 960-2
- [68] Jean P, Martin M and Lecler D 1967 *C. R. Séances Acad. Sci. Ser. B* **264** 1709-12
- [69] Henderson M and Curtis L J 1996 *J. Phys. B: At. Mol. Opt. Phys.* **29** L629-34
- [70] Ansbacher W, Pinnington E H and Kernahan J A 1988 *Can. J. Phys.* **66** 402-4
- [71] Ansbacher W, Pinnington E H, Tauheed A and Kernahan J A 1989 *Phys. Scr.* **40** 454-6
- [72] Frage S, Karwowski J and Saxena K M A 1976 *Handbook of Atomic Data* Elsivier, Amsterdam
- [73] Cowan R D 1981 *The Theory of Atomic Structure and Spectra* (Univ. California Press, Berkeley)
- [74] Biémont E, Garnir H P, Palmeri P, Li Z S and Svanberg S 2000 *Mon. Not. R. Astron. Soc.* **312** 116-22
- [75] Henderson M, Curtis L J, Matulioniene R, Ellis D G and Theodosiou C E 1997 *Phys. Rev. A* **56** 1872-8
- [76] Norby L J 1991 *J. Chem. Edu.* **68** 110-3
- [77] Pyykkö P 1988 *Chemical Reviews* **88** 563-94