Energy differences and magnetic dipole ($M1$) decay rates for the W^{52+} and Bi^{61+} members of the nearly-Z-independent $(3d_{3/2})^3 3d_{5/2}$ $J=3-J=2$ transition

Donald R. Beck
Physics Department, Michigan Technological University, Houghton, Michigan 49931
(Received 2 June 1999)

Relativistic configuration-interaction results have been obtained for the $(3d_{3/2})^3 3d_{5/2}$ $J=3 \rightarrow J=2$ transition in W^{52+} and Bi^{61+}. If prior work on Gd^{42+}, Nd^{38+}, Ba^{34+}, and Xe^{32+} is a guide, the accuracy of our results should be in the 1–2 % range. Both these species have recently been under active experimental study. The transition itself is thought to provide a very useful plasma diagnostic tool because it lies in the optical region, and is remarkably constant with Z. [S1050-2947(99)06010-2]

PACS number(s): 31.25.Eb, 31.25.Jf, 31.30.Jv, 32.30.Jc

I. INTRODUCTION

In 1991, Feldman *et al.* [1] performed Dirac-Fock (DF) calculations for $M1$ rates and energy differences among levels of $2p^k$, $3p^k$, and $3d^l$ ground configurations (closed shells had been deleted). They were looking at highly ionized species, such as are found in plasmas, and seeking transition energies (and intensities) that might be observed using optical means. All transitions but one were either found to be too energetic (i.e., nonoptical) or the initial state too highly excited (weakly populated or having a more rapid decay channel). The sole exception they found was the $(3d_{3/2})^3 3d_{5/2}$ $J=3 \rightarrow J=2$ transition, which had the unusual feature that the energy difference was nearly constant with Z, thus potentially allowing this line to act as a diagnostic for a great variety of plasma ions. Specifically, the wavelength of the line changes about 14% in going from $Z=54$ (Xe) to $Z=82$ (Pb). The work of Feldman *et al.* [1] included DF energy differences and $M1$ decay rates (for both the $J=3 \rightarrow J=2$ and $J=3 \rightarrow J=4$ transitions, where appropriate, for selected members of the isoelectronic sequence).

In 1995, Morgan *et al.* [2] experimentally observed the line in Ba^{34+} and Xe^{32+}, and in 1996, Serpa *et al.* [3] observed it in Nd^{38+} and Gd^{42+}. The Feldman *et al.* [1] energy differences were found to be $\sim$5% ($\sim$1360 cm^{-1}) too high and Indelicato [4] tried to improve these results by including some unspecified valence-shell and core correlations, with little success. As part of his work, he found a second nearly Z-independent transition for $(4d_{3/2})^3 4d_{5/2}$ $J=3 \rightarrow J=2$ (energy difference $\sim$13.340 cm^{-1} for W^{52+}) and a less constant one in $4f^6 J=4 \rightarrow J=5$, but neither of these is in the optical regime.

In 1997, Beck [5] was able to reduce the error in energy differences to 1–2 % for the four measured wavelengths; the 1% value was associated with the more thorough calculations (Gd^{42+}), through a systematic inclusion of correlation effects, using relativistic configuration interaction. Since that time, requests have been made by experimenters [6,7] for results for W^{52+} and Bi^{61+}, and we report these results here. Hopefully they will also be at the 1–2 % level, which is still a competitive accuracy.

II. THEORY AND RESULTS

The zeroth-order function is generated by solving the Dirac-Fock-Coulomb equations for the $3d^4$ levels, using the computer program of Desclaux [8]. Output also includes evaluation of the Breit operator, both magnetic and retardation parts, using first order perturbation theory, and an estimate of radiative effects, using the Welton picture [8]. This function includes all relativistic configurations associated with the $3d^4$ nonrelativistic manifold, even though one, the $(3d_{3/2})^3 3d_{5/2}$, is dominant ($>$95%).

Correlation effects are included by making single and double excitations from the $n=3$ subshells of the $1s^2 2s^2 2p^6 3s^2 3p^6 3d^4$ nonrelativistic manifold. The radial parts of the unoccupied subshells are represented by relativistic screened hydrogenic functions, with $n=l+1$, whose exponents (Z^*) are determined as part of the relativistic configuration interaction energy variational process. Further details of the method will be found in Ref. [5], and the references cited therein.

Results for the W^{52+} and Bi^{61+} energy differences are given in Table I. Our prediction of 27 766 cm for W^{52+} is 434 cm^{-1} lower than the prediction of Feldman *et al.* [1],

TABLE I. Contributions (in cm-1) to the $(3d_{3/2})^3 3d_{5/2}$ $J=3-J=2$ energy difference.

Origin	Bi^{61+}	W^{52+}
Dirac-Coulomb	30 598	29 053
$3s \rightarrow 3d$	-299	-331
$3p^2 \rightarrow 3d^2$	$+1095$	$+855$
$3s^2 \rightarrow 3d^2$	-14	-21
$3d \rightarrow vd$	-2	-18
$3d \rightarrow vg$	-69	-95
$3d \rightarrow vi$	-19	-19
$3p \rightarrow vp$	$+102$	$+121$
$3p \rightarrow vf$	-997	-880
$3p \rightarrow vh$	-30	-24
$3s \rightarrow vd$	-18	-18
Total correlation	-251	-430
Magnetic	-1256	-849
Retardation	$+6$	$+5$
Radiative	-12	-13
Misc.	-29	
Total (this work)	29 056	27 766
Other theory [1]		28 200

TABLE II. $M1$ transition rates for decay of $(3d_{3/2})^3 3d_{5/2}$ $J_k=3$ to $(3d_{3/2})^3 3d_{5/2}$ J_i.

Species	dE (a.u.)	A_{ki} $(J_i=2)$	dE (a.u.)	A_{ki} $(J_i=4)$
W^{52+} (this work)	0.12651	246 s^{-1}	0.244 47	1231 s^{-1}
W^{52+} (Feldman *et al.* [1])	0.12849	263 s^{-1}	0.255 07	1424 s^{-1}
Bi^{61+} (this work)	0.13240	234 s^{-1}	0.272 71	1505 s^{-1}

and presumably [5] closer to the experimental value, which will be reported shortly [7]. For the three elements: Xe^{32+}, Nd^{38+}, and W^{52+}, calculated by both Feldman *et al.* [1] and this author, the change in energy difference seems to be entirely due to correlation effects, as might be expected. Errors for the first two species are 4.7% and 5.5% for Feldman *et al.* [1], whereas for Beck [5] the errors are 1.4% and 2.0%.

Several qualitative observations may be made. From Table I, we see that the most important corrections to the Dirac-Fock-Coulomb result come from the magnetic Breit (i.e., there is a strong level dependence) and the $3p^2 \rightarrow 3d^2$ and $3p \rightarrow vf$ correlation effects, which act in opposite directions.

Comparing Table I of this work, with Table I of the earlier work [5], one notes that there is a strong Z dependence of magnetic Breit, $3p^2 \rightarrow 3d^2$ and $3p \rightarrow vf$ contributions. It should also be noted that the total correlation contribution declines significantly as Z increases, which tends to improve the relative accuracy of the multiconfigurational Dirac-Fock results (with nonaverage Breit included).

The entry Misc. in Table I, for Bi^{61+}, is a total of the number of correlation effects too small to list explicitly. These include the following: $3d^2 \rightarrow vf^2(E+M) + vd^2(E+M) + vdvg(E) + vsvg(E) + vfvh(E) + vdvi(E) + vgvi(E)$; $3p^2 \rightarrow 3dvd(E+M) + 3dvg(E)$; $2p \rightarrow vp + vf(E+M)$; $2p^2 \rightarrow 3d^2(E)$; $2p3p \rightarrow 3d^2(E)$, and $2s \rightarrow 3d(E)$. Here, E means the Coulomb Hamiltonian, and M means that the magnetic Breit effect is included. The triple and quadruple excitations $3p^3 \rightarrow 3d^2vf$ and $3p^4 \rightarrow 3d^4$ were also investigated for Bi^{61+} $J=3$, but as these effects were small (~ 130 cm^{-1}), they were not included in the energy difference. Because of the small size of the Misc. contributions, they were not included for W^{52+}. A similar approach was taken for Gd^{42+} in the earlier work [5].

In Table II, $M1$ transition rates are reported for W^{52+} and Bi^{61+} for the $J=3 \rightarrow J=2$ and $J=3 \rightarrow J=4$ branches. These were calculated with program RFE [9], which includes the effect of nonorthonormality. There is little difference between the correlated and Dirac-Fock-Coulomb values, and the difference between the values of Table II and those of Feldman *et al.* [1] for W^{52+} is mostly due to the different wavelengths used. The Bi^{61+} values reported in Table II were calculated by Norquist [10], who also obtained $E2$ rates for the $J=3$ level. These have not been reported as they are much smaller than the $M1$ rates.

ACKNOWLEDGMENT

I thank the Division of Chemical Sciences, Office of Energy Research, U.S. Department of Energy, Grant No. DE-FG02-92ER14282, for support of this work.

[1] U. Feldman, P. Indelicato, and J. Sugar, J. Opt. Soc. Am. B **8**, 3 (1991).
[2] C. A. Morgan, F. G. Serpa, E. Takacs, E. S. Meyer, J. D. Gillaspy, J. Sugar, J. R. Roberts, C. M. Brown, and U. Feldman, Phys. Rev. Lett. **74**, 1716 (1995).
[3] F. G. Serpa, E. S. Meyer, C. A. Morgan, J. D. Gillaspy, J. Sugar, J. R. Roberts, C. M. Brown, and U. Feldman, Phys. Rev. A **53**, 2220 (1996).
[4] P. Indelicato, Phys. Scr. **T65**, 57 (1996).
[5] D. R. Beck, Phys. Rev. A **56**, 2428 (1997).
[6] G. Serpa (private communication).
[7] J. D. Gillaspy (private communication).
[8] J. P. Desclaux, Comput. Phys. Commun. **9**, 31 (1975).
[9] D. R. Beck, Program RFE (unpublished).
[10] P. L. Norquist (private communication).