Energy levels and radiative rates for Br-like ions with $Z \leq 50$

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INTRODUCTION

Atomic data for energy levels and radiative rates (A-values) are required for the modelling of fusion plasmas for a range of elements and their ions. Laboratory measurements for a few energy levels are generally available, but the corresponding data for the A- values are very limited. Therefore, we have recently reported such data for a few Br-like ions, namely with $38 \leq Z \leq 42$ [1] and W XL [2]. Here we extend the work for 8 other ions with $43 \leq Z \leq 50$, or specifically Tc IX, Ru X, Rh XI, Pd XII, Ag XIII, Cd XIV, In XV, and Sn XVI.

CALCULATIONS

We have adopted the General-purpose Relativistic Atomic Structure Package (GRASP) code and have calculated A- values for the electric dipole (E1), electric quadrupole (E2), magnetic dipole (M1), and magnetic quadrupole (M2) transitions. Extensive CI (configuration interaction) among 39 configurations is included, i.e. $4s^24p^5$, $4s^24p^44d/4f$, $4s4p^6$, $4p^64d/4f$, $4s4p^54d/4f$, $4s^24p^34d^2/4f^2/4d4f$, $4s^24p^24d^3$, $4s^24p4d^4$, $4s^24p^24d^24f$, $4s4p^34d^3$, $4p^54d^2$, $3d^94s^24p^54d/4f$, $3d^94s^24p^6$, $4s4p^55\ell$, $4p^65\ell$, $4s^24p^45\ell$, and $3d^94s^24p^55\ell$. These configurations generate 3990 levels in total and have been carefully chosen, because of their interacting energy ranges. Other configurations, such as $3p^53d^{10}4s^24p^6$, $3p^53d^{10}4s^24p^54d$ and $3p^53d^{10}4s^24p^54f$, have also been tested, but excluded from the calculations because they generate levels at much higher energy ranges, and hence their impact on the lower energy levels is insignificant. This has been confirmed by performing considerably larger calculations with the *Flexible Atomic Code* (FAC), which involve 12,137 levels. The additional 8147 levels have arisen from the inclusion of the $4p^6$ 6*1, $4s4p^5$ 6*1, $4s^24p^4$ 6*1, $4p^6$ 7*1, $4s4p^5$ 7*1, $4s^24p^4$ 7*1, $3p^53d^{10}4s^24p^6$, $3p^53d^{10}4s^24p^5$ 4d/4f, $4s^24p^3$ 5*2, and $4s4p^4$ 5*2 configurations.

RESULTS

Energies, A- values and lifetimes (τ) have been determined for 3990 levels for all 8 Br-like ions. Since experimental energies are available only for the levels of the $4s^24p^5$ and $4s^24p^45s$ configurations, we compare our results in Tables 1–3 for Ru X, Rh XI and Pd XII. In general, our energies with the GRASP code are higher than the measurements by up to 4%, and those obtained with FAC show even (*slightly*) larger discrepancies. This indicates that the additional CI included in FAC is of no advantage as far as the levels of the $4s^24p^45s$ configuration are concerned. However, it may be possible to improve upon the accuracy of our calculated energies by including a significantly larger CI (i.e. thousands of configurations generating over a million levels).

Wavelengths (λ) in ~ 10 Å range for 13 transitions of Sn XVI between the levels of the $4s^24p^44d$ and $4s^24p^45p$ configurations have been measured by D'Arcy et al. [3] who also reported the f- values. Agreement with our calculations with GRASP is within 3% for the wavelengths but differences for the f- values are up to 50% for a few. However, all measured lines are weak, i.e. $f \leq 0.1$, for which differing amount of CI produce variable results.

TABLE 1: COMPARISON OF ENERGIES (cm^{-1}) FOR SOME LEVELS OF RU X.

Index	Configuration	Level	EXPT	GRASP	FAC	% (GRASP-EXPT)
1	$4s^24p^5$	$^2P_{3/2}$	0	0	0	0.0
2	$4s^24p^5$	$^2P_{1/2}$	33055	32475	32692	1.8
3	$4s^24p^45s$	$^4P_{5/2}$	697786	722065	722882	3.5
4	$4s^24p^45s$	$^4P_{3/2}$	704647	730991	731173	3.8
5	$4s^24p^45s$	$^4P_{1/2}$	719748	743827	755756	3.3
6	$4s^24p^45s$	$^2P_{3/2}$	728687	753451	753958	3.4
7	$4s^24p^45s$	$^2P_{1/2}$	734754	761299	761226	3.6
8	$4s^24p^45s$	$^2D_{5/2}$	745861	774115	774251	3.8
9	$4s^24p^45s$	$^2D_{3/2}$	747170	775688	775703	3.8
10	$4s^24p^45s$	$^2S_{1/2}$		816576	817660	

TABLE 2: COMPARISON OF ENERGIES (cm^{-1}) FOR SOME LEVELS OF RH XI.

Index	Configuration	Level	EXPT	GRASP	FAC	% (GRASP-EXPT)
1	$4s^24p^5$	$^2P_{3/2}$	0	0	0	0.0
2	$4s^24p^5$	$^2P_{1/2}$	38800	38207	38427	1.5
3	$4s^24p^45s$	$^4P_{5/2}$	793311	819083	820088	3.2
4	$4s^24p^45s$	$^4P_{3/2}$	800634	828596	828928	3.5
5	$4s^24p^45s$	$^4P_{1/2}$	817622	843153	844236	3.1
6	$4s^24p^45s$	$^2P_{3/2}$	829627	855780	856496	3.2
7	$4s^24p^45s$	$^2P_{1/2}$	835880	863940	864045	3.4
8	$4s^24p^45s$	$^2D_{5/2}$	847458	877288	877651	3.5
9	$4s^24p^45s$	$^2D_{3/2}$		879140	879361	
10	$4s^24p^45s$	$^2S_{1/2}$		925392	926577	

TABLE 3: COMPARISON OF ENERGIES (cm^{-1}) FOR SOME LEVELS OF PD XII.

Index	Configuration	Level	EXPT	GRASP	FAC	% (GRASP-EXPT)
1	$4s^24p^5$	$^2P_{3/2}$	0	0	0	0.0
2	$4s^24p^5$	$^2P_{1/2}$	45180	44589	44815	1.3
3	$4s^24p^45s$	$^4P_{5/2}$	893577	920763	921902	3.0
4	$4s^24p^45s$	$^4P_{3/2}$	901344	930820	930820	3.3
5	$4s^24p^45s$	$^4P_{1/2}$	920125	947077	948265	2.9
6	$4s^24p^45s$	$^2P_{3/2}$	935948	963428	964300	2.9
7	$4s^24p^45s$	$^2P_{1/2}$	942450	971900	972139	3.1
8	$4s^24p^45s$	$^2D_{5/2}$	954474	985758	986294	3.3
9	$4s^24p^45s$	$^2D_{3/2}$	956353	987896	988270	3.3
10	$4s^24p^45s$	$^2S_{1/2}$		1040196	1041450	

EXPT: M Even-Zohar and BS Fraenkel, J.Phys. **B 5** (1972) 1596
GRASP: present calculations from the GRASP code with 3990 levels
FAC: present calculations from the FAC code with 12,137 levels

CONCLUSIONS

1. Based on limited comparisons with available measurements and our calculations with two independent atomic codes (GRASP and FAC), and with differing amount of CI, our energy levels are assessed to be accurate to better than 4%, although scope remains for improvements.

2. Corresponding available results for f- values are limited to only 13 transitions of Sn XVI for which differences with our calculations are up to 50% for a few. However, all such transitions are *weak* and therefore it is difficult to assess their accuracy based on such limited comparisons.

3. Presented results are *preliminary* and their detailed analysis is still in progress.

REFERENCES

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2. KM Aggarwal and FP Keenan, *ADNDT* **100** (2014) 1399

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