

Energy levels, radiative rates, and lifetimes for Br-like ions with $Z \geq 38$

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Atomic Parameters

- ENERGY LEVELS

$$E_j - E_i = h\nu_{ij} = hc/\lambda_{ij}$$

- RADIATIVE RATES (A , s^{-1}),
OSCILLATOR STRENGTHS (f , dimensionless),
LINE STRENGTHS (S , a.u.)

$$f_{i,j} = \frac{mc}{8\pi^2 e^2} \lambda_{ji}^2 \frac{\omega_j}{\omega_i} A_{ji} = 1.49 \times 10^{-16} \lambda_{ji}^2 \frac{\omega_j}{\omega_i} A_{ji}$$
$$E1 : A_{ji} = \frac{2.0261 \times 10^{18}}{\omega_j \lambda_{ji}^3} S \text{ and } f_{ij} = \frac{303.75}{\lambda_{ji} \omega_i} S,$$
$$E2 : A_{ji} = \frac{1.1199 \times 10^{18}}{\omega_j \lambda_{ji}^5} S \text{ and } f_{ij} = \frac{167.89}{\lambda_{ji}^3 \omega_i} S,$$
$$M1 : A_{ji} = \frac{2.6974 \times 10^{13}}{\omega_j \lambda_{ji}^3} S \text{ and } f_{ij} = \frac{4.044 \times 10^{-3}}{\lambda_{ji} \omega_i} S,$$
$$M2 : A_{ji} = \frac{1.4910 \times 10^{13}}{\omega_j \lambda_{ji}^5} S \text{ and } f_{ij} = \frac{2.236 \times 10^{-3}}{\lambda_{ji}^3 \omega_i} S.$$

λ is in Å.



Sr IV (Z=38)

Y V (Z=39)

Zr VI (Z=40)

Nb VII (Z=41)

Mo VII (Z=42)

39 configurations, i.e. $4s^2 4p^5$, $4s^2 4p^4 4d$, $4s 4p^6$, $4p^6 4d/4f$, $4s^2 4p^4 4f$,
 $4s 4p^5 4d/4f$, $4s^2 4p^3 4f^2/4d^2/4d 4f$, $4s^2 4p^2 4d^3$, $4s^2 4p 4d^4$, $4s^2 4p^2 4d^2 4f$,
 $4s 4p^3 4d^3$, $4p^5 4d^2$, $3d^9 4s^2 4p^5 4d/4f$, $3d^9 4s^2 4p^6$, $4s 4p^5 5l$, $4p^6 5l$,
 $4s^2 4p^4 5l$, and $3d^9 4s^2 4p^5 5l$ **total 3990 levels**

W XL (Z=74)

46 configurations, i.e. $4s^2 4p^5$, $4s^2 4p^4 4d$, $4s^2 4p^4 4f$, $4s 4p^6$,
 $3d^9 4s^2 4p^6$, $4p^6 4d/4f$, $4s 4p^5 4d/4f$, $4p^3 4d^2/4f^2/4d 4f$, $4s^2 4p^2 4d^3$,
 $4s^2 4p 4d^4$, $4s^2 4p^2 4d^2 4f$, $4s 4p^3 4d^3$, $4p^5 4d^2$, $3d^9 4s^2 4p^5 4d/4f$,
 $3p^5 3d^{10} 4s^2 4p^6$, $3p^5 3d^{10} 4s^2 4p^5 4d/4f$, $4s 4p^5 5l$, $4p^6 5l$, $4s^2 4p^4 5l$,
 $3d^9 4s^2 4p^5 5l$, and $(4s^2 4p^4) 6s/6p/6d/6f$ **total 4128 levels**



1 GRASP0

PH Norrington

<http://web.am.qub.ac.uk/DARC/>

2 FAC

MF Gu, Can J. Phys. **86** (2008) 675

<http://sprg.ssl.berkeley.edu/~mfgu/fac/>

Configurations for W XL

Index	Configuration	No. of Levels	Energy Range (Ryd)	GRASP1	GRASP2	RELAC
1	$4s^2 4p^5$	2^o	0–7	Y	Y	Y
2	$4s^2 4p^4 4d$	28	11–27	Y	Y	Y
3	$4s^2 4p^4 4f$	30^o	25–42	Y	Y	Y
4	$4s 4p^6$	1	15	Y	Y	Y
5	$4p^6 4d$	2	43–45	Y	Y	
6	$4p^6 4f$	2^o	58–59	Y	Y	
7	$4s 4p^5 4d$	23^o	25–36	Y	Y	Y
8	$4s 4p^5 4f$	24	41–50	Y	Y	Y
9	$4s^2 4p^3 4d^2$	141^o	22–42	Y	Y	
10	$4s^2 4p^3 4f^2$	221^o	52–71	Y	Y	
11	$4s^2 4p^3 4d 4f$	363	37–58	Y	Y	
12	$4s^2 4p^2 4d^3$	261	34–57	Y	Y	
13	$4s^2 4p 4d^4$	180^o	54–73	Y	Y	
14	$4s^2 4p^2 4d^2 4f$	1140^o	49–73	Y	Y	
15	$4s 4p^3 4d^3$	678^o	47–73	Y	Y	
16	$4p^5 4d^2$	45^o	53–64	Y	Y	
17	$3d^9 4s^2 4p^5 4d$	96^o	131–147	Y	Y	Y
18	$3d^9 4s^2 4p^5 4f$	113	147–161	Y	Y	Y
19	$3d^9 4s^2 4p^6$	2	120–126	Y	Y	Y
20	$3p^5 3d^{10} 4s^2 4p^6$	2^o	155–178	Y	Y	Y
21	$3p^5 3d^{10} 4s^2 4p^5 4d$	65	165–198	Y	Y	Y
22	$3p^5 3d^{10} 4s^2 4p^5 4f$	36^o	180–212	Y	Y	Y



Configurations for W XL ... cont.

Index	Configuration	No. of Levels	Energy Range (Ryd)	GRASP1	GRASP2	RELAC
23	4s4p ⁵ 5s	7 ^o	65–74	Y	Y	
24	4s4p ⁵ 5p	18	68–80	Y	Y	
25	4s4p ⁵ 5d	23 ^o	77–86	Y	Y	
26	4s4p ⁵ 5f	24	84–92	Y	Y	
27	4s4p ⁵ 5g	24 ^o	87–96	Y	Y	
28	4p ⁶ 5s	1	82	Y	Y	
29	4p ⁶ 5p	2 ^o	86–89	Y	Y	
30	4p ⁶ 5d	2	94–95	Y	Y	
31	4p ⁶ 5f	2 ^o	100–101	Y	Y	
32	4p ⁶ 5g	2	104–105	Y	Y	
33	4s ² 4p ⁴ 5s	8	50–65	Y	Y	Y
34	4s ² 4p ⁴ 5p	21 ^o	54–72	Y	Y	Y
35	4s ² 4p ⁴ 5d	28	62–78	Y	Y	Y
36	4s ² 4p ⁴ 5f	30 ^o	69–84	Y	Y	Y
37	4s ² 4p ⁴ 5g	30	73–88	Y	Y	
38	3d ⁹ 4s ² 4p ⁵ 5s	23 ^o	172–185	Y	Y	Y
39	3d ⁹ 4s ² 4p ⁵ 5p	65	175–191	Y	Y	Y
40	3d ⁹ 4s ² 4p ⁵ 5d	96 ^o	183–197	Y	Y	Y
41	3d ⁹ 4s ² 4p ⁵ 5f	113	190–203	Y	Y	Y
42	3d ⁹ 4s ² 4p ⁵ 5g	119 ^o	194–207	Y	Y	
43	4s ² 4p ⁴ 6s	8	81–96		Y	
44	4s ² 4p ⁴ 6p	21 ^o	81–99		Y	
45	4s ² 4p ⁴ 6d	28	87–102		Y	
46	4s ² 4p ⁴ 6f	30 ^o	91–106		Y	

GRASP1 and GRASP2: Calculations with 4128 levels and 4215 levels, respectively
 RELAC: Fournier, ADNDT 68 (1998) 1 [only 10 even and 10 odd configurations](#)



Mixing coefficients for levels of W XL

Index	Configuration	Level	Mixing coefficients
1	4s ² 4p ⁵	² P _{3/2} ^o	0.99(1)
2	4s ² 4p ⁵	² P _{1/2} ^o	0.99(2)
3	4s ² 4p ⁴ (³ P)4d	⁴ D _{3/2}	-0.61(3)+0.43(12)-0.29(28)+0.44(16)-0.26(20)-0.23(7)
4	4s ² 4p ⁴ (³ P)4d	⁴ P _{1/2}	0.37(15)-0.68(4)-0.24(9)+0.45(29)-0.32(23)
5	4s ² 4p ⁴ (³ P)4d	⁴ D _{5/2}	-0.35(17) 0.66(5)-0.26(11)+0.26(21)+0.40(13)-0.33(26)
6	4s ² 4p ⁴ (³ P)4d	⁴ F _{7/2}	0.56(6)-0.31(19)+0.52(8)+0.52(18)-0.20(27)
7	4s ² 4p ⁴ (¹ S)4d	² D _{3/2}	0.44(60)+0.33(12)+0.23(28)+0.21(22)+0.74(7)
8	4s ² 4p ⁴ (³ P)4d	² F _{7/2}	0.65(19)+0.51(8)+0.25(18)+0.47(27)
9	4s ² 4p ⁴ (³ P)4d	² P _{1/2}	0.25(15)+0.27(4)-0.60(9)+0.36(29)+0.48(23)-0.38(14)
10	4s ² 4p ⁴ (³ P)4d	⁴ F _{9/2}	0.83(10)+0.55(24)
11	4s ² 4p ⁴ (³ P)4d	⁴ P _{5/2}	0.25(17)+0.46(11)-0.39(25)+0.71(66)
12	4s ² 4p ⁴ (³ P)4d	⁴ P _{3/2}	0.26(60)-0.49(12)-0.42(28)+0.42(22)+0.40(16)+0.38(20)
13	4s ² 4p ⁴ (¹ D)4d	² F _{5/2}	-0.35(17)-0.39(5)+0.26(11)-0.22(25)+0.48(21)+0.43(13)+0.30(26)-0.32(66)
14	4s4p ⁶	² S _{1/2}	0.45(4)-0.28(9)+0.82(14)
15	4s ² 4p ⁴ (³ P)4d	⁴ D _{1/2}	-0.89(15)-0.31(9)+0.27(29)
16	4s ² 4p ⁴ (¹ D)4d	² D _{3/2}	-0.53(60)+0.58(3)+0.21(12)+0.35(22)+0.31(16)-0.30(20)
17	4s ² 4p ⁴ (³ P)4d	⁴ F _{5/2}	0.68(17)+0.35(25)+0.27(21)+0.50(13)-0.26(26)
18	4s ² 4p ⁴ (¹ D)4d	² G _{7/2}	0.37(6)+0.40(8)-0.77(18)+0.29(27)
19	4s ² 4p ⁴ (³ P)4d	⁴ D _{7/2}	0.62(6)+0.65(19)-0.33(8)-0.27(27)
20	4s ² 4p ⁴ (¹ D)4d	² P _{3/2}	-0.61(12)-0.74(20)
21	4s ² 4p ⁴ (³ P)4d	² D _{5/2}	0.27(17)+0.28(5)-0.29(11)+0.60(21)-0.43(13)+0.44(26)
22	4s ² 4p ⁴ (³ P)4d	² P _{3/2}	-0.32(60)-0.37(3)+ 0.69(22)-0.50(16)
...			

Energy levels of W XL (in Ryd)

Index	Configuration	Level	NIST	GRASP1	GRASP2	FAC1	FAC2	RELAC
1	4s ² 4p ⁵	² P _{3/2} ^o	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	4s ² 4p ⁵	² P _{1/2} ^o	6.7632	6.8419	6.7980	6.8104	6.8102	6.8213
3	4s ² 4p ⁴ (³ P)4d	⁴ D _{3/2}		11.0344	11.2569	11.2699	11.2780	11.0971
4	4s ² 4p ⁴ (³ P)4d	⁴ D _{5/2}		11.2042	11.4241	11.4371	11.4450	11.2652
5	4s ² 4p ⁴ (³ P)4d	⁴ P _{1/2}	11.2290	11.2068	11.4280	11.4398	11.4475	11.2788
6	4s ² 4p ⁴ (³ P)4d	⁴ F _{7/2}	11.4100	11.4084	11.6105	11.6220	11.6296	11.4609
7	4s ² 4p ⁴ (¹ S)4d	² D _{3/2}		12.0304	12.1503	12.1597	12.1673	12.0890
8	4s ² 4p ⁴ (³ P)4d	² F _{7/2}	12.5338	12.5350	12.7466	12.7644	12.7724	12.5901
9	4s ² 4p ⁴ (³ P)4d	² P _{1/2}	12.5852	12.5745	12.8145	12.8296	12.8367	12.6535
10	4s ² 4p ⁴ (³ P)4d	⁴ F _{9/2}		12.6163	12.8113	12.8290	12.8369	12.6604
11	4s ² 4p ⁴ (³ P)4d	⁴ P _{5/2}		13.6091	13.7413	13.7548	13.7621	13.6743
12	4s ² 4p ⁴ (³ P)4d	⁴ P _{3/2}	13.8791	13.9843	14.0922	14.1067	14.1136	14.0390
13	4s ² 4p ⁴ (¹ D)4d	² F _{5/2}	14.0930	14.2332	14.3243	14.3387	14.3457	14.2659
14	4s4p ⁶	² S _{1/2}	14.9266	15.0298	15.3667	15.3781	15.3795	15.0905
...								

GRASP1: present calculations from the GRASP code with 63 levels

GRASP2: present calculations from the GRASP code with 4128 levels

FAC1: present calculations from the FAC code with 4128 levels

FAC2: present calculations from the FAC code with 11,525 levels

RELAC: Fournier, ADNDT 68 (1998) 1

NIST energies are uncertain by up to 0.05 Ryd but additional CI makes the comparison worse

Aggarwal & Keenan, Can. J. Phys. **92** (2014) 545



Comparison of f- values for some transitions of W XL.

I	J	GRASP1	GRASP3	FAC1	FAC2	GRASP4	RELAC	R3	R4
1	3	2.724-3	3.047-3	3.071-3	3.073-3	2.780-3	2.903-3	7.3-1	9.2-1
1	4	1.929-3	2.255-3	2.302-3	2.315-3	1.830-3	2.377-3	7.4-1	9.3-1
1	5	6.938-3	6.545-3	6.453-3	6.450-3	5.600-3	7.760-3	8.0-1	9.5-1
1	7	2.236-4	3.027-4	3.161-4	3.166-4	2.130-4	1.148-4	8.7-1	1.1-0
1	9	3.192-3	3.178-3	2.786-3	2.748-3	1.690-3	3.865-3	1.0-0	1.1-0
1	11	5.333-6	3.228-3	3.169-3	3.105-3	1.440-3	3.798-5	9.0-1	1.0-0
1	12	2.891-1	2.652-1	2.670-1	2.673-1	2.590-1	3.018-1	7.9-1	9.5-1
1	13	5.990-1	5.187-1	5.225-1	5.232-1	5.130-1	5.633-1	8.0-1	9.6-1
1	14	1.887-1	1.523-1	1.563-1	1.567-1	1.620-1	1.585-1	7.2-1	9.2-1
1	15	1.365-3	1.289-3	1.272-3	1.269-3	1.240-3	7.5-1	9.1-1
1	16	1.757-4	1.340-4	1.358-4	1.380-4	1.010-4	9.3-1	1.1-0
1	17	2.684-2	2.683-2	2.657-2	2.662-2	2.510-2	2.885-2	8.4-1	9.7-1
1	20	7.276-2	2.461-1	2.617-1	2.639-1	6.630-2	9.385-2	8.4-1	9.5-1
1	22	2.747-3	9.173-1	9.251-1	9.262-1	2.860-3	1.018-0	8.4-1	9.7-1
1	23	1.063-0	2.784-2	2.029-2	1.993-2	9.350-1	1.210-2	8.6-1	9.7-1
1	24	5.970-1	3.158-1	3.011-1	2.993-1	5.380-1	5.843-1	8.4-1	9.6-1
1	25	5.270-1	4.261-1	4.232-1	4.231-1	4.430-1	4.730-1	8.1-1	9.5-1
1	26	1.511-1	2.747-2	2.646-2	2.613-2	1.130-1	9.165-2	8.3-1	9.7-1
1	28	4.291-2	3.220-2	3.171-2	3.168-2	3.540-2	8.5-1	9.7-1
1	29	6.720-5	2.096-4	1.350-4	1.268-4	1.680-4	1.8-1	1.6-0
1	30	8.904-5	1.945-6	2.020-6	9.7-1	1.1-0
1	31	3.429-4	5.839-4	5.745-4	5.716-4	5.860-4	7.7-1	9.8-1

GRASP1: present calculations from the GRASP code with 63 levels

GRASP3: present calculations from the GRASP code with 4128 levels **R3**

FAC1: present calculations from the FAC code with 4128 levels

FAC2: present calculations from the FAC code with 11,525 levels

GRASP4: 638 level calculation of S. Aggarwal et al, Can J. Phys. 91 (2013) 394 **R4**

RELAC: Fournier, ADNDT 68 (1998) 1

Calculations with large CI are consistent but differ considerably with others

Aggarwal & Keenan, Can. J. Phys. **92** (2014) 545



Comparison of W XL lifetimes (τ , s).

Index	Configuration	Level	GRASP3	GRASP4a	GRASP4b	GRASP4a (Dominant A- values, s ⁻¹)
2	4s ² 4p ⁵	² P _{1/2} ^o	1.314-07	1.312-07	1.37-07	1-2 M1=7.29+06
3	4s ² 4p ⁴ (³ P)4d	⁴ D _{3/2}	3.218-10	3.422-10	3.43-10	1-3 E1=2.92+09
6	4s ² 4p ⁴ (³ P)4d	⁴ F _{7/2}	4.765-03	4.119-03	6.07-03	1-6 M2=1.64+02, 4-6 M1=7.84+01
7	4s ² 4p ⁴ (¹ S)4d	² D _{3/2}	2.692-09	3.595-09	3.82-09	1-7 E1=2.62+08
8	4s ² 4p ⁴ (³ P)4d	² F _{7/2}	2.238-05	2.209-05	8.00-05	1-8 M2=1.25+04, 4-8 M1=2.44+04
9	4s ² 4p ⁴ (³ P)4d	² P _{1/2}	1.046-10	1.633-10	2.18-10	1-9 E1=4.56+09, 2-9 E1=1.56+09
10	4s ² 4p ⁴ (³ P)4d	⁴ F _{9/2}	3.703-05	3.731-05	1.27-01	6-10 M1=2.68+04
16	4s ² 4p ⁴ (³ P)4d	⁴ F _{3/2}	5.133-10	5.615-10	3.73-09	2-16 E1=1.51+09
17	4s ² 4p ⁴ (³ P)4d	⁴ F _{5/2}	2.070-11	2.165-11	2.16-11	1-17 E1= 4.62+10
18	4s ² 4p ⁴ (¹ D)4d	² G _{7/2}	2.604-07	2.554-07	4.74-04	6-18 M1=3.03+6
19	4s ² 4p ⁴ (³ P)4d	⁴ D _{7/2}	1.356-07	1.349-07	7.91-05	8-19 M1=2.09+06, 10-19 M1=2.99+06
20	4s ² 4p ⁴ (¹ D)4d	² P _{3/2}	1.317-12	4.736-12	4.77-12	1-20 E1=2.11+11
21	4s ² 4p ⁴ (¹ D)4d	² G _{9/2}	2.445-07	2.404-07	8.39-05	10-21 M1=3.10+06
27	4s ² 4p ⁴ (¹ D)4d	² F _{7/2}	2.046-07	2.018-07	6.41-04	10-27 M1=2.69+06
29	4s ² 4p ⁴ (¹ D)4d	² P _{1/2}	7.449-13	6.751-13	7.47-10	2-29 E1=1.48+12
30	4s ² 4p ⁴ (³ P)4d	² D _{3/2}	6.228-13	5.512-13	8.66-08	2-30 E1=1.81+12

GRASP3: present calculations from the GRASP code with 4128 levels

GRASP4a: present calculations from the GRASP code with 638 levels

GRASP4b: 638 level calculation of S. Aggarwal et al, Can. J. Phys. 91 (2013) 394

GRASP4b τ differ by over 5 orders of magnitude
 Aggarwal & Keenan, Can. J. Phys. 92 (2014) 545



Configurations for Br-like ions

Index	Configuration	No. of Level	Sr IV	Y V	Zr VI	Nb VII	Mo VIII
1	4s ² 4p ⁵	2 ^o	0.0 – 0.1	0.0 – 0.1	0.0 – 0.1	0.0 – 0.2	0.0 – 0.2
2	4s ² 4p ⁴ 4d	28	1.8 – 2.6	2.1 – 3.0	2.4 – 3.5	2.7 – 3.9	3.0 – 4.3
3	4s ² 4p ⁴ 4f	30 ^o	3.1 – 3.5	3.8 – 4.3	4.6 – 5.2	5.2 – 5.9	5.8 – 6.9
4	4s4p ⁶	1	1.5 – 1.5	1.7 – 1.7	1.9 – 1.9	2.1 – 2.1	2.3 – 2.3
5	4p ⁶ 4d	2	5.5 – 5.5	6.4 – 6.4	6.9 – 7.2	7.5 – 8.2	8.2 – 9.1
6	4p ⁶ 4f	2 ^o	6.9 – 7.0	8.1 – 8.4	9.3 – 9.6	10.3 – 10.8	11.8 – 12.1
7	4s4p ⁵ 4d	23 ^o	3.1 – 3.6	3.6 – 4.3	4.0 – 5.1	4.5 – 5.7	5.1 – 5.9
8	4s4p ⁵ 4f	24	4.6 – 5.7	5.5 – 6.9	6.5 – 8.0	7.4 – 8.1	8.3 – 9.0
9	4s ² 4p ³ 4d ²	141 ^o	3.6 – 5.0	4.1 – 5.7	4.7 – 6.6	5.2 – 7.4	5.8 – 8.1
10	4s ² 4p ³ 4f ²	221 ^o	6.5 – 7.2	8.0 – 8.6	9.4 – 10.3	10.7 – 11.8	12.0 – 13.6
11	4s ² 4p ³ 4d4f	363	4.9 – 6.1	6.0 – 7.3	7.0 – 8.6	8.0 – 9.9	8.9 – 11.4
12	4s ² 4p ² 4d ³	261	5.7 – 7.3	6.5 – 8.6	7.4 – 9.8	8.1 – 11.0	9.0 – 12.2
13	4s ² 4p4d ⁴	180 ^o	8.2 – 9.7	9.5 – 11.3	10.8 – 12.9	11.8 – 14.4	13.1 – 16.0
14	4s ² 4p ² 4d ² 4f	1140 ^o	7.0 – 8.5	8.3 – 10.2	9.5 – 11.6	10.7 – 13.4	11.9 – 15.2
15	4s4p ³ 4d ³	678 ^o	6.5 – 9.2	7.4 – 10.7	8.4 – 12.2	9.3 – 13.7	10.3 – 15.1
16	4p ⁵ 4d ²	45 ^o	6.8 – 7.5	7.7 – 8.4	8.7 – 9.6	9.6 – 10.8	10.6 – 11.8
17	3d ⁹ 4s ² 4p ⁵ 4d	96 ^o	10.3 – 11.4	12.1 – 13.4	13.9 – 15.5	15.9 – 17.7	17.9 – 19.9
18	3d ⁹ 4s ² 4p ⁵ 4f	113	11.8 – 12.1	14.1 – 14.5	16.4 – 16.9	18.8 – 19.5	21.2 – 22.1
19	3d ⁹ 4s ² 4p ⁶	2	8.4 – 8.6	9.9 – 10.1	11.5 – 11.7	13.2 – 13.4	15.0 – 15.2
20	4s4p ⁵ 5s	7 ^o	3.8 – 4.4	4.6 – 5.3	5.3 – 6.2	6.3 – 7.2	7.3 – 8.2
21	4s4p ⁵ 5p	18	4.1 – 4.8	5.0 – 5.8	5.9 – 6.8	6.9 – 7.8	7.9 – 9.0
22	4s4p ⁵ 5d	23 ^o	4.6 – 5.3	5.7 – 6.4	6.8 – 7.6	7.9 – 8.8	9.1 – 10.1
23	4s4p ⁵ 5f	24	5.1 – 5.7	6.3 – 7.0	7.5 – 8.3	8.8 – 9.7	10.2 – 11.1
24	4s4p ⁵ 5g	24 ^o	5.1 – 5.7	6.4 – 7.0	7.7 – 8.4	9.1 – 9.9	10.5 – 11.4



Configurations for Br-like ions ... cont.

Index	Configuration	No. of Level	Sr IV	Y V	Zr VI	Nb VII	Mo VIII
25	4p ⁶ 5s	1	6.0 – 6.0	7.1 – 7.1	8.2 – 8.2	9.3 – 9.3	10.5 – 10.5
26	4p ⁶ 5p	2 ^o	6.3 – 6.3	7.4 – 7.6	8.7 – 8.7	9.8 – 10.0	11.1 – 11.2
27	4p ⁶ 5d	2	6.9 – 6.9	8.1 – 8.1	9.5 – 9.5	10.9 – 10.9	12.3 – 12.3
28	4p ⁶ 5f	2 ^o	7.2 – 7.3	8.7 – 8.7	10.2 – 10.3	11.7 – 11.8	13.4 – 13.5
29	4p ⁶ 5g	2	7.3 – 7.3	8.8 – 8.8	10.4 – 10.4	12.0 – 12.0	13.7 – 13.7
30	4s ² 4p ⁴ 5s	8	2.2 – 2.6	2.8 – 3.3	3.5 – 4.0	4.2 – 4.8	4.9 – 5.6
31	4s ² 4p ⁴ 5p	21 ^o	2.5 – 2.9	3.2 – 3.7	4.0 – 4.6	4.8 – 5.4	5.6 – 6.4
32	4s ² 4p ⁴ 5d	28	3.0 – 3.5	3.9 – 4.4	4.8 – 5.4	5.8 – 6.4	6.8 – 7.5
33	4s ² 4p ⁴ 5f	30 ^o	3.5 – 3.9	4.5 – 4.9	5.4 – 6.2	6.7 – 7.4	7.8 – 8.6
34	4s ² 4p ⁴ 5g	30	3.5 – 3.9	4.6 – 5.0	5.7 – 6.2	6.9 – 7.5	8.1 – 8.8
35	3d ⁹ 4s ² 4p ⁵ 5s	23 ^o	10.8 – 11.2	12.9 – 13.3	15.2 – 15.7	17.6 – 18.1	20.1 – 20.7
36	3d ⁹ 4s ² 4p ⁵ 5p	65	11.1 – 11.7	13.3 – 14.0	15.7 – 16.4	18.2 – 19.0	20.8 – 21.7
37	3d ⁹ 4s ² 4p ⁵ 5d	96 ^o	11.7 – 12.1	14.1 – 14.6	16.6 – 17.2	19.2 – 19.9	22.0 – 22.8
38	3d ⁹ 4s ² 4p ⁵ 5f	113	12.2 – 12.5	14.7 – 15.1	17.4 – 17.8	20.2 – 20.7	23.1 – 23.7
39	3d ⁹ 4s ² 4p ⁵ 5g	119 ^o	12.2 – 12.5	14.8 – 15.2	17.5 – 18.0	20.4 – 20.9	23.4 – 24.0



Energies (Ryd) for the levels of Mo VIII.

Index	Configuration	Level	NIST	GRASP2a	GRASP2b	GRASP3	FAC1	FAC2	FAC3
1	4s ² 4p ⁵	² P _{3/2} ^o	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
2	4s ² 4p ⁵	² P _{1/2} ^o	0.21209	0.20770	0.20676	0.20776	0.21363	0.20913	0.20962
3	4s4p ⁶	² S _{1/2}	2.13082	2.12679	2.27306	2.25774	2.28111	2.31642	2.31460
4	4s ² 4p ⁴ (³ P)4d	⁴ D _{5/2}	2.81307	2.79438	2.94319	2.88062	2.95802	2.95864	2.95659
5	4s ² 4p ⁴ (³ P)4d	⁴ D _{7/2}		2.80088	2.94980	2.88823	2.96622	2.96738	2.96505
6	4s ² 4p ⁴ (³ P)4d	⁴ D _{3/2}	2.82436	2.80908	2.95788	2.89461	2.97206	2.97229	2.97051
7	4s ² 4p ⁴ (³ P)4d	⁴ D _{1/2}		2.83678	2.98561	2.92291	3.00109	3.00186	3.00021
8	4s ² 4p ⁴ (³ P)4d	⁴ F _{9/2}		2.94108	3.09038	3.02231	3.09862	3.09795	3.09621
9	4s ² 4p ⁴ (³ P)4d	⁴ F _{7/2}		3.00278	3.15221	3.08273	3.15778	3.15727	3.15638
10	4s ² 4p ⁴ (¹ D)4d	² P _{1/2}	3.01450	3.04338	3.19233	3.12243	3.19970	3.19842	3.19928
12	4s ² 4p ⁴ (³ P)4d	⁴ F _{3/2}	3.05879	3.07138	3.22305	3.13829	3.22889	3.21173	3.21195
11	4s ² 4p ⁴ (³ P)4d	⁴ F _{5/2}	3.07954	3.10018	3.22072	3.14797	3.23226	3.22651	3.22557
13	4s ² 4p ⁴ (³ P)4d	⁴ P _{1/2}	3.07039	3.07388	3.24975	3.17990	3.25085	3.25444	3.25614
14	4s ² 4p ⁴ (³ P)4d	⁴ P _{3/2}	3.09398	3.10968	3.25906	3.18700	3.26494	3.26378	3.26468
15	4s ² 4p ⁴ (¹ D)4d	² D _{3/2}	3.11072	3.13738	3.28654	3.21432	3.29200	3.29015	3.29142
...									

GRASP2a: 470 level calculations of Singh *et al* [Phys. Scr. 88 (2013) 035301]

GRASP2b: present calculations from the GRASP code with 470 levels

GRASP3: present calculations from the GRASP code with 3990 levels

FAC1: present calculations from the FAC code with 470 levels

FAC2: present calculations from the FAC code with 3990 levels

FAC3: present calculations from the FAC code with 12,137 levels

With the same CI, FAC and GRASP agree, but results of Singh et al differ by up to 0.15 Ryd

and cannot be reproduced



Comparison of radiative rates (A- values, s^{-1}) and oscillator strengths (f- values) for E1 transitions of Zr VI

Transition		GRASP2a		GRASP2b			GRASP3		Ratio
I	J	A	f	A	f	A	f		
1	3	5.30+08	1.11-02	1.2340+09	2.2440-02	1.0518+09	1.9249-02	4.4-1	
1	4	1.17+07	4.44-04	1.5391+07	5.1968-04	2.0308+07	7.0217-04	9.4-1	
1	6	7.76+06	1.94-04	9.2931+06	2.0713-04	1.1017+07	2.5149-04	9.8-1	
1	7	4.75+06	5.83-05	5.3458+06	5.8707-05	5.6982+06	6.4052-05	9.8-1	
1	10	1.28+07	1.35-04	1.4776+07	1.4070-04	2.1200+08	6.1728-03	9.6-1	
1	11	1.41+08	4.42-03	1.4199+08	4.0235-03	1.0789+07	1.0527-04	1.4-0	
1	12	3.35+05	6.96-06	1.0270+06	1.9240-05	5.1806+05	1.0018-05	9.2-1	
1	13	4.67+08	4.76-03	4.7004+08	4.3119-03	5.9759+08	5.6133-03	8.0-1	
1	14	5.50+08	1.12-02	4.8841+08	8.9413-03	7.0038+08	1.3157-02	9.8-1	
1	15	3.37+08	6.71-03	2.5187+08	4.5310-03	2.5390+08	4.6958-03	9.1-1	
1	17	1.60+08	4.66-03	1.1567+08	3.0399-03	1.5603+08	4.2219-03	8.3-1	
1	18	6.97+07	1.34-03	6.2901+07	1.0945-03	1.7608+07	3.1416-04	1.3-0	
1	19	3.82+08	1.08-02	2.5563+08	6.5103-03	2.6359+08	6.8923-03	9.8-1	
1	22	1.96+08	5.33-03	1.4639+08	3.6141-03	3.0306+08	7.6802-03	1.0-0	
1	23	3.24+08	7.92-03	3.1381+08	6.9890-03	3.9608+08	9.0568-03	8.2-1	
1	25	1.68+09	2.36-02	1.4350+09	1.8453-02	4.0018+09	5.5609-02	9.9-1	
1	26	3.16+02	6.43-09	2.1868+07	4.0909-04	2.1104+09	4.2754-02	1.1-0	
1	27	1.56+11	1.85-00	1.3479+11	1.4662-00	1.2527+11	1.5107-00	9.3-1	
1	28	1.63+11	9.52-01	1.5331+11	8.2221-01	9.7116+10	5.7290-01	9.0-1	
1	29	1.91+11	3.25-00	1.0623+10	5.5136-02	6.3978+10	3.5747-01	8.0-1	
1	30	1.29+10	7.24-02	1.7896+11	2.7997-00	1.6154+11	2.8075-00	9.1-1	
1	31	7.17+09	7.55-02	7.6240+09	7.3961-02	7.1045+09	7.6658-02	8.8-1	
2	3	2.40+08	1.18-02	5.3588+08	2.2736-02	4.7253+08	2.0219-02	4.1-1	
2	6	3.21+05	1.82-05	1.0080+03	5.0645-08	1.2890-00	6.6505-11	1.2+3	
...									

A- values of Singh et al differ by up to 5 orders of magnitude
and cannot be reproduced



Comparison of lifetimes (τ , s) for the levels of Zr VI

Index	Configuration	Level	GRASP2a	GRASP2b	GRASP3	GRASP2b (dominant A- values, s ⁻¹)
1	4s ² 4p ⁵	² P _{3/2} ^o
2	4s ² 4p ⁵	² P _{1/2} ^o	1.47-02	1.630-02	1.583-02	1 - 2 M1 = 6.126+01
3	4s4p ⁶	² S _{1/2}	6.31-10	5.650-10	6.560-10	1 - 3 E1 = 1.234+09, 2 - 3 E1 = 5.359+08
7	4s ² 4p ⁴ (³ P)4d	⁴ D _{1/2}	1.91-07	9.679-08	9.501-08	1 - 7 E1 = 5.346+06, 2 - 7 E1 = 4.986+06
8	4s ² 4p ⁴ (³ P)4d	⁴ F _{9/2}	9.02+01	2.876-01	3.117-01	5 - 8 M1 = 3.468+00
9	4s ² 4p ⁴ (³ P)4d	⁴ F _{7/2}	1.80-01	8.920-02	9.182-02	1 - 9 M2 = 3.848+00, 5 - 9 M1 = 3.250+00, 8 -
10	4s ² 4p ⁴ (¹ D)4d	² P _{1/2}	1.81-07	1.150-08	4.717-09	2 - 10 E1 = 7.218+07
11	4s ² 4p ⁴ (³ P)4d	⁴ F _{5/2}	5.83-09	7.043-09	1.401-08	1 - 11 E1 = 1.420+08
12	4s ² 4p ⁴ (³ P)4d	⁴ F _{3/2}	6.16-08	2.081-08	1.916-08	2 - 12 E1 = 4.704+07
15	4s ² 4p ⁴ (¹ D)4d	² D _{3/2}	3.16-09	1.882-09	1.529-09	1 - 15 E1 = 2.519+08, 2 - 15 E1 = 2.795+08
16	4s ² 4p ⁴ (³ P)4d	² F _{7/2}	4.11-01	2.171-02	2.241-02	5 - 16 M1 = 1.845+01, 8 - 16 M1 = 1.447+01
20	4s ² 4p ⁴ (¹ D)4d	² G _{7/2}	2.42-01	1.810-02	1.879-02	5 - 20 M1 = 1.393+01, 9 - 20 M1 = 2.029+01
21	4s ² 4p ⁴ (¹ D)4d	² G _{9/2}	9.88+00	1.609-02	1.686-02	8 - 21 M1 = 4.981+01
24	4s ² 4p ⁴ (¹ D)4d	² F _{7/2}	2.26-00	7.230-03	7.502-03	5 - 24 M1 = 4.515+01, 8 - 24 M1 = 5.213+01
25	4s ² 4p ⁴ (¹ S)4d	² D _{3/2}	6.89-10	3.240-10	2.128-10	1 - 25 E1 = 1.435+09, 2 - 25 E1 = 1.651+09
26	4s ² 4p ⁴ (¹ S)4d	² D _{5/2}	1.26-04	4.573-08	4.738-10	1 - 26 E1 = 2.187+07
...						

τ - values of Singh et al differ by up to 4 orders of magnitude
and cannot be reproduced



Conclusions

- Results of energy levels, radiative rates and lifetimes reported by Singh *et al* [Phys. Scr. **88** (2013) 035301] for Br-like ions **cannot be reproduced**. Although energies differ by only up to 0.15 Ryd, A and τ differ by up to **5 orders of magnitude**.
- Improvements and extensions have been made over the available atomic data for Br-like ions,
- but scope remains for further improvements.
- Detailed results along with comparisons will soon be available in Phys. Scr. **89** (2014) 000000

