Excitation

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Boron

Neutral B RMPS finished (just).

3 active electrons $\rightarrow$ 640 CC.

Ballance, Griffin, Berrington & Badnell:

JPB to be submitted.

B isonuclear sequence finished (finally).

B^{+} (NRB, DM, DCG) - 134 CC: JPB 36, 1337 (2003)

B^{2+} (NRB and Dmitri Borodin) - RMPS as per other Li-like (in ADAS)

B^{3+} (CPB) - n=5 RMPS (unpublished)

B^{4+} (CPB) - n=5 RMPS JPB 36, 3707 (2003)

DARC/BPRM

DARC: Ni-like W (Ballance & Griffin JPB v39 3617, 2006) identical approach to Ni-like Xe (Badnell et al JPB v37 4589, 2004). Also, Cu- and Zn-like Ballance et al JPB submitted.

DARC Ne-like Fe (reported by Connor last year) published Loch et al JPB v39, 85 (2006)

DARC and BPRM for Mg-like Fe: Berrington et al JPB v38, 1667 (2005).

Used same CI expansion, with orbitals optimized in the same way.

Used same CC expansion.

Used same energy mesh resolution for resonances.

Differences in upsilons consistent with uncertainties in target description and resonance resolution, i.e. nothing attributable to Dirac vs BP Hamiltonians per se.

$Z = 26$ and $\alpha = 1/137$, so . . .

Recall:

Both DARC and BPRM include one-body operators

$\alpha^2 Z^n$

where $n = 4$ for b-b, $n = 3$ for b-c and $n = 2$ for c-c.

DARC omits Breit interaction.

Two-body fine-structure is (being) incorporated into BPRM (Eissner et al).

$Z^2\Omega \sim A + \alpha^2 Z^2 B + \alpha^4 Z^4 C + \ldots$

AS, ICFTR and heavy species

From Jonauskas et al JPB v38 L79 (2005), +ICR. Energy levels in W^{70+}.

Index	Level		IC(FT)	RHF	DARC	RI	ICR
1	2s2	1S0	-14472.2313	-14606.1630	-14661.2007	-14661.2127	-14660.1972
2	2s12p1	3P0	11.8033	9.5122	12.7642	13.3690	12.4027
3	2s12p1	3P1	14.4817	12.5698	15.6393	16.3163	15.4486
4	2p2	3P0	32.9833	29.5304	35.8501	36.6611	35.0358
5	2s12p1	3P2	101.4780	125.3516	123.2548	122.9797	123.2114
6	2s12p1	1P1	107.3621	131.9927	129.7459	129.3913	129.8507
7	2p2	3P1	119.6724	141.7643	142.9160	143.2261	142.6208
8	2p2	1D2	121.6674	143.8498	144.8975	145.2266	144.7094
9	2p2	3P2	210.3791	258.4229	254.3276	253.8651	254.5042
10	2p2	1S0	214.6380	262.8561	258.6676	258.1166	258.9496

The RI method takes radial integrals from GRASP/DARC and averages over kappa and feeds them back into "BP" RM. Here RI is RM-ICFT structure but with relativistic integrals. The ICR aproach averages the orbitals over kappa, then does the integrals. More elegant, but I have not gotten around to coding the relativistic continuum basis in "BP" RM. ICFT RM less computationally demanding than BP/DARC. Interest to extend via "ICFTR".