Atomic and Molecular Data Update - USA

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Excitation and Charge Transfer in Ion-Atom Collisions

- TD Lattice, AOCC, and CTMC calculations for
    - $p + H^*$
    - $\alpha + H$
    - $Be^{4+} + H$
    - $p + He^+$

T Lee, T Minami, DR Schultz, and MS Pindzola
      *PRA **72**, 062703 (2005)*
*T Minami, MS Pindzola, T Lee, and DR Schultz, JPB **39**, 2877 (2006)*

Excitation in Electron-Atom Collisions

- Semi-relativistic RMPS and fully relativistic RM calculations.

  - e + He
  - e + B, e + B^{3+} (All B ions now have RMPS excitation data).
  - e + W^{44+}, e + W^{45+}, e + W^{46+}

CP Ballance, DC Griffin, SD Loch, RF Boivin, and MS Pindzola
      *PRA **74**, 012719 (2006)*
*CP Ballance and DC Griffin JPB **39**, 3617 (2006)*

Ionization in Electron-Atom Collisions

- RMPS, TDCC, DW and CTMC calculations
  - e + H* ions [RMPS, TDCC]
  - e + He-like ions (Li$^+$, B^{3+}, C^{4+}) [RMPS]
  - e + Be-like ions (C^{2+}, N^{3+}, O^{4+}) [RMPS]
  - e + Ar [RMPS]
  - e + W^{q+} (all ion stages) [CADW]
  - e + Ar^{q+} (all ion stages) [CADW]

e + Ar ionization calculation using RMPS
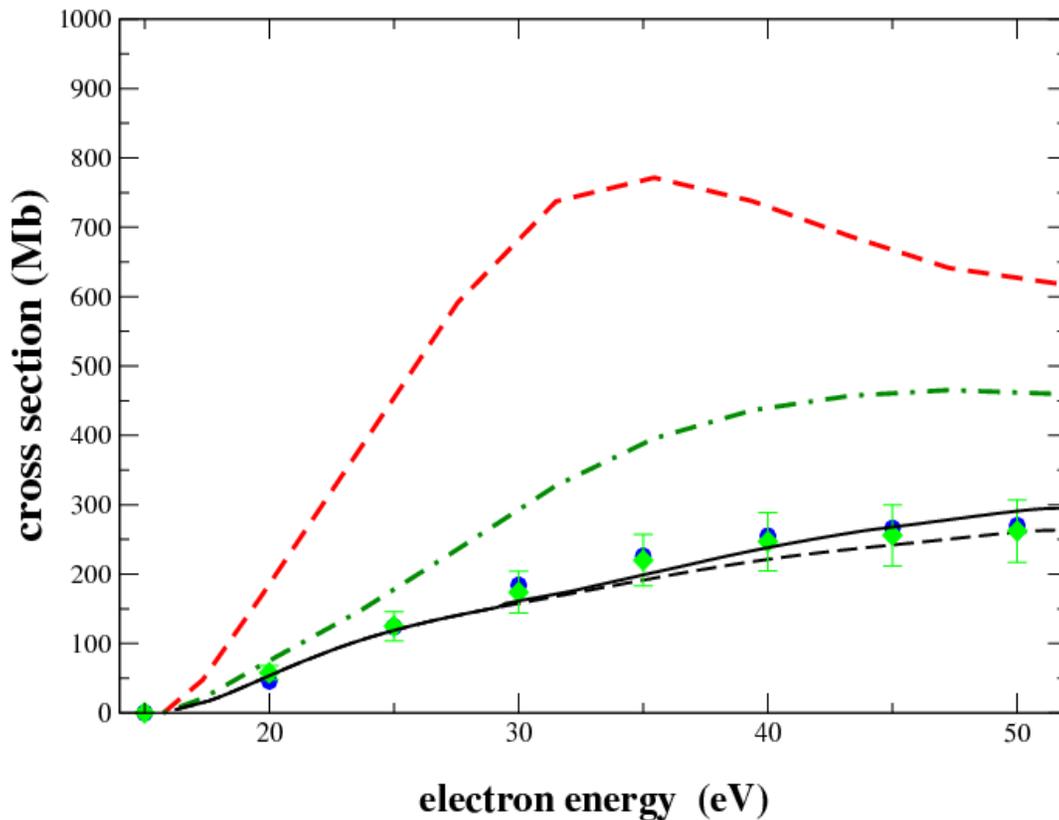
- Red dashed line shows the CADW results.

- Green dot-dashed line shows the term resolved DW results.

- Black dashed line shows the RMPS results.

- Solid black line shows the RMPS results with ionization from the 3s included using the CADW method.

- The experiments of Straub et al. (1995) and Wetzel et al. (1987) are also shown.

Automated checking of CADW ionization data – Example for Tungsten
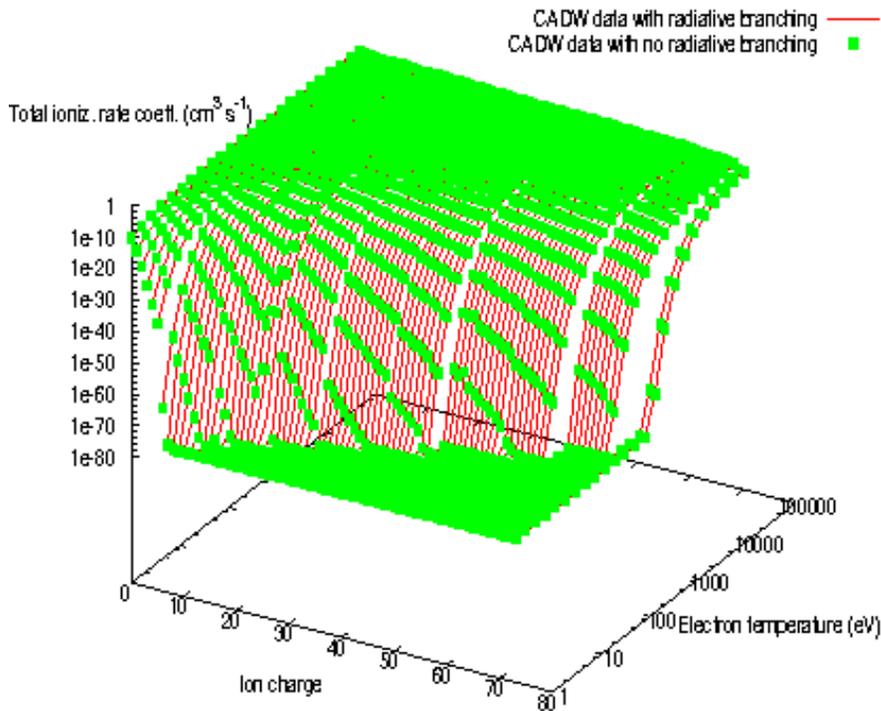
We plot the old and new total rate coefficient data to check for obvious differences/errors.
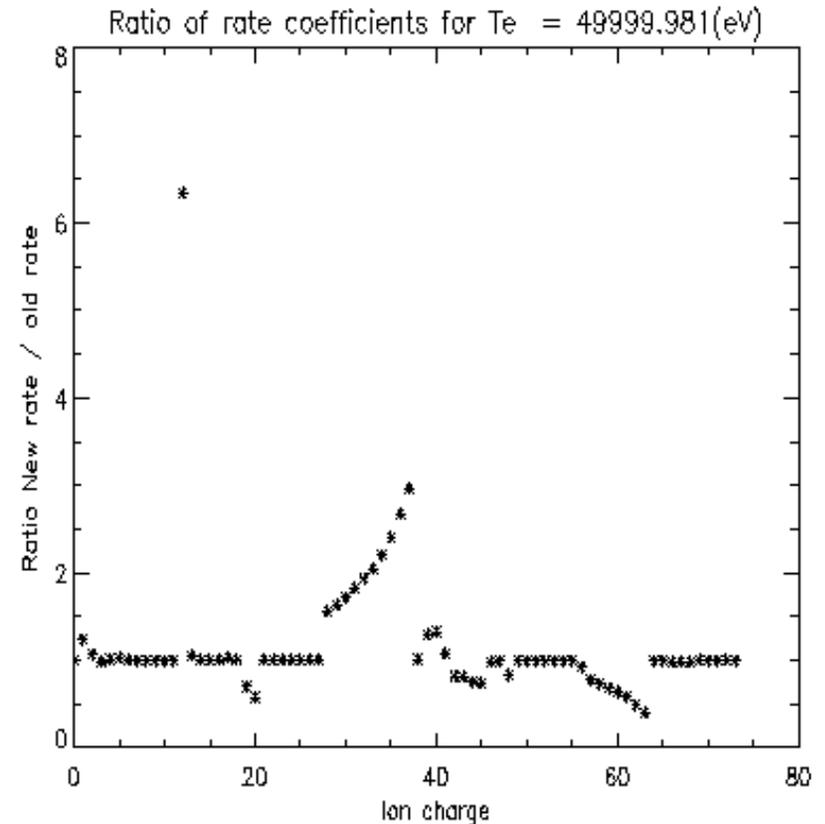
The ratio of new/old data as a function of ion charge is more revealing. The effects of including the 3d direct ionization can be seen on W^{27+}-W^{37+}, and an error in the old datafile for W^{12+} is also seen.

Ionization in Electron-Molecule Collisions

- TDCC and DW calculations for
  - e + H_2^+
  - e + H_2

MS Pindzola, FJ Robicheaux, and JP Colgan,
   *JPB **38**, 4285 (2005)*
MS Pindzola, FJ Robicheaux, and JP Colgan,
   *PRA **73**, 052706 (2006)*

New Calculations

- e + C, C$^+$ excitation with RMPS.
- e + Mo$^+$ ionization with RMPS.
- e + Ar$^+$ excitation with RMPS.
- α + Li^{2+} with TD lattice.
- e + Li^{+*} ionization with TDCC.
- e + Xe and e + Mo all ion stages CADW.

Code Development

- RMPS for double ionization.
- TDCC for fast ion-He collisions.
- Parallelizing LSJ-level resolved DW for excitation-autoionization.
- TDCC cylindrical for p + H, p + He.
- TDCC spherical with HF core for e + Ar ionizaton.