Modified Relativistic Approach for Atomic Data Calculation

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Outlook

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1. Relativistic integral analogues
   - Method
   - Changes to standard R-matrix codes
   - Results
2. Quasirelativistic Hartree-Fock Approach
   - Method
   - Energy Level Spectra
   - Transition Line Spectra

Outlook

Relativistic Integral Analogues

- A relation for multipole integral

$$M^k(n_1 l_1, n_2 l_2) = \frac{1}{2} \sum_{j_1 j_2} [j_1, j_2] \left\{ \begin{array}{ccc} j_1 & j_2 & k \\ l_2 & l_1 & 1/2 \end{array} \right\}^2 M^k(n_1 l_1 j_1, n_2 l_2 j_2)$$

- A non-relativistic multipole integral

$$M^k(n_1 l_1, n_2 l_2) = \int_0^\infty dr\ P_{n_1 l_1}\ r^k\ P_{n_2 l_2}$$

- A relativistic multipole integral

$$M^k(n_1 l_1 j_1, n_2 l_2 j_2) = \int_0^\infty dr\ r^k \left[P_{n_1 l_1 j_1}\ P_{n_2 l_2 j_2} + Q_{n_1 \bar{l}_1 j_1}\ Q_{n_2 \bar{l}_2 j_2} \right]$$

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Relativistic Integral Analogues

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$$M^k(n_1 l_1, n_2 l_2) = \frac{1}{2} \sum_{j_1 j_2} [j_1, j_2] \begin{Bmatrix} j_1 & j_2 & k \\ l_2 & l_1 & 1/2 \end{Bmatrix}^2 M^k(n_1 l_1 j_1, n_2 l_2 j_2)$$

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Outlook

Changes in standard R-matrix codes

Amendments to R-matrix flow

- Start from relativistic R-matrix version (DARC)
  GRASP $\rightarrow$ DSTG0 $\rightarrow$ DSTG1/ORB/INT
- Follow with non-relativistic R-matrix (RmaX)
  AUTOSTRUCTURE $\rightarrow$ STG1 $\rightarrow$STG2 $\rightarrow$ STGH
- Finish with intermediate coupling frame transformation method (ICFT)
  STGICF $\rightarrow$ STGF
- Test on electron-impact excitation of $2s^2$ - $2s2p\ ^3S^1$ transition

  V.Jonauskas et al., J.Phys B **38** *(2005) L79-L85*

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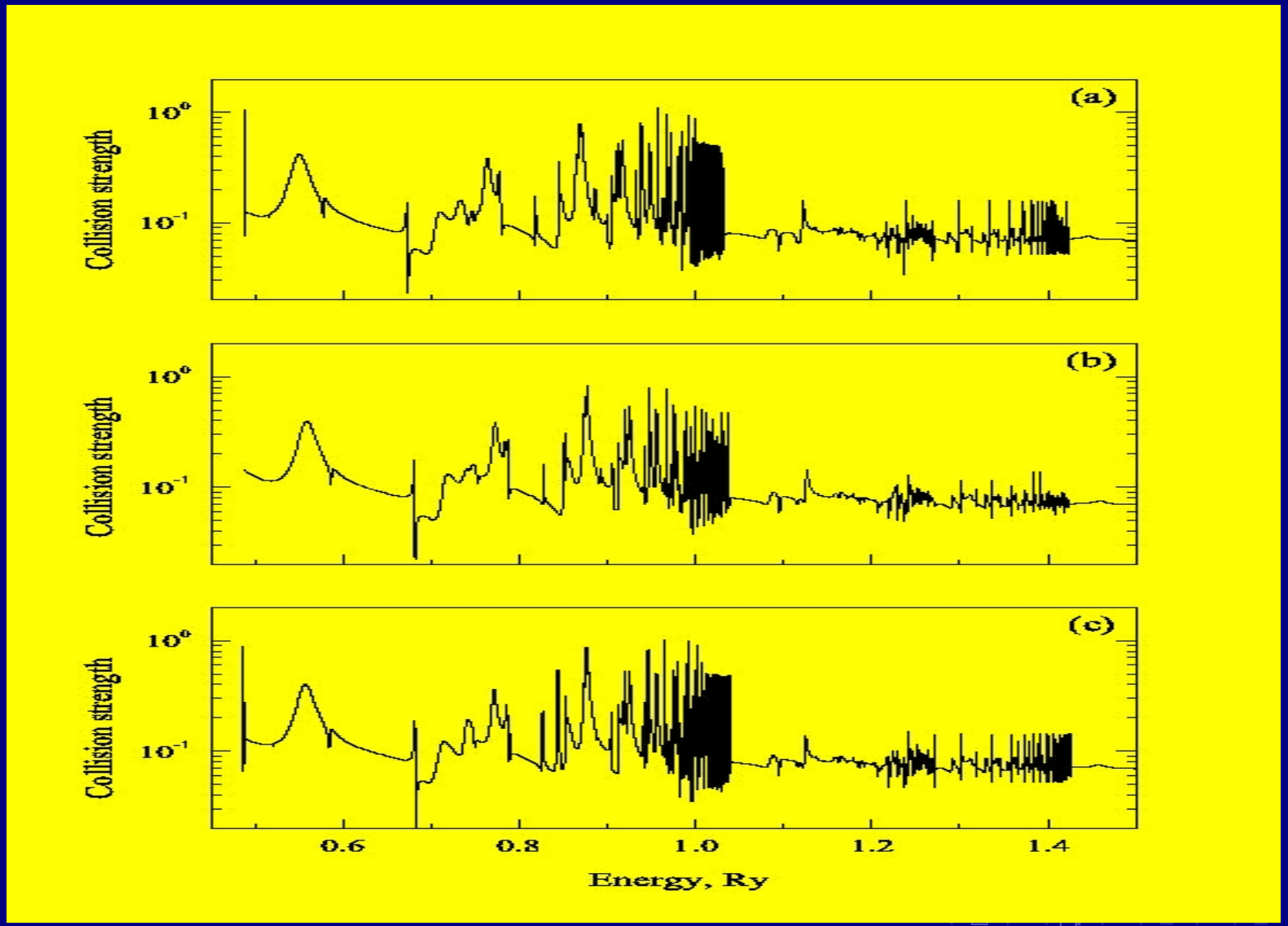
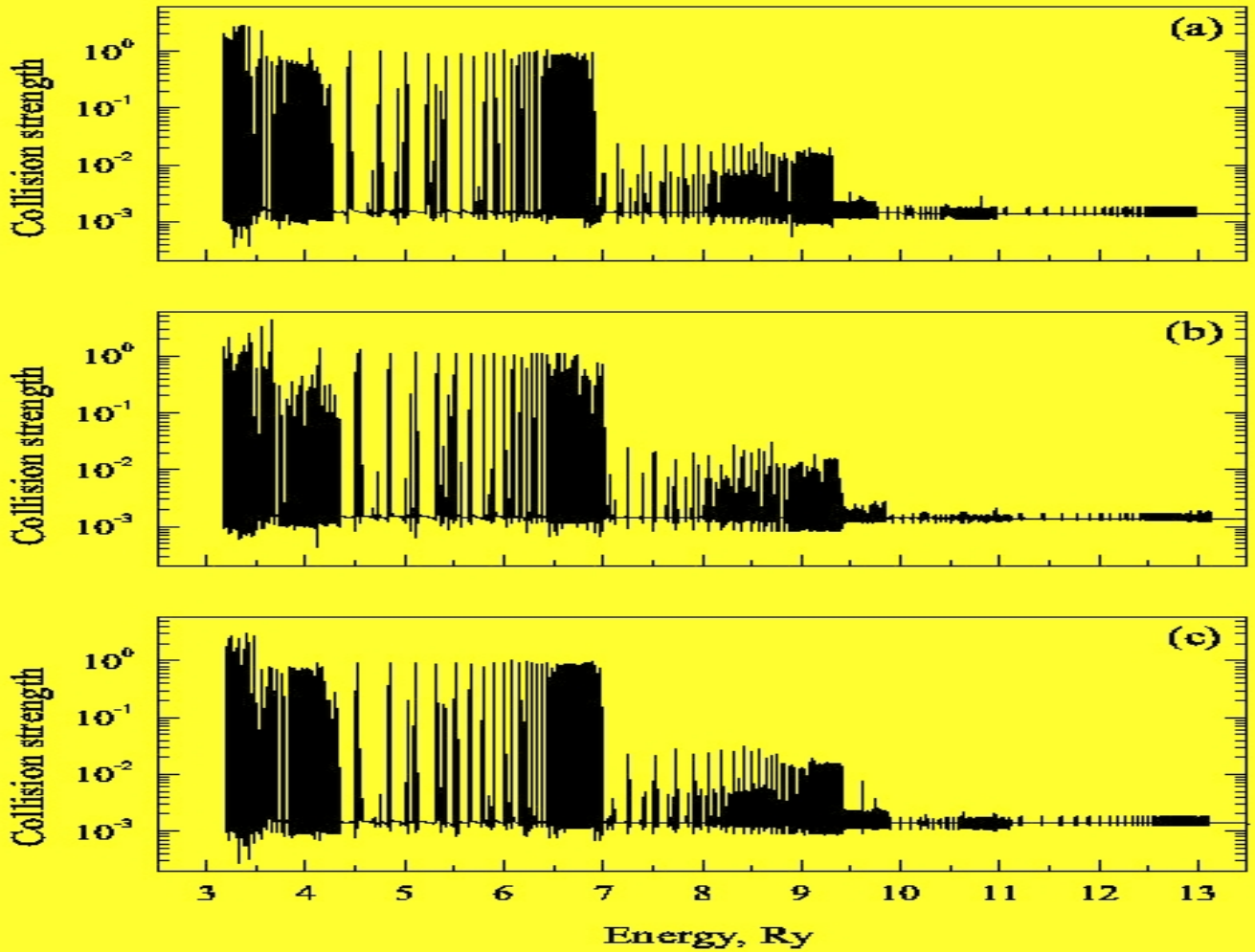
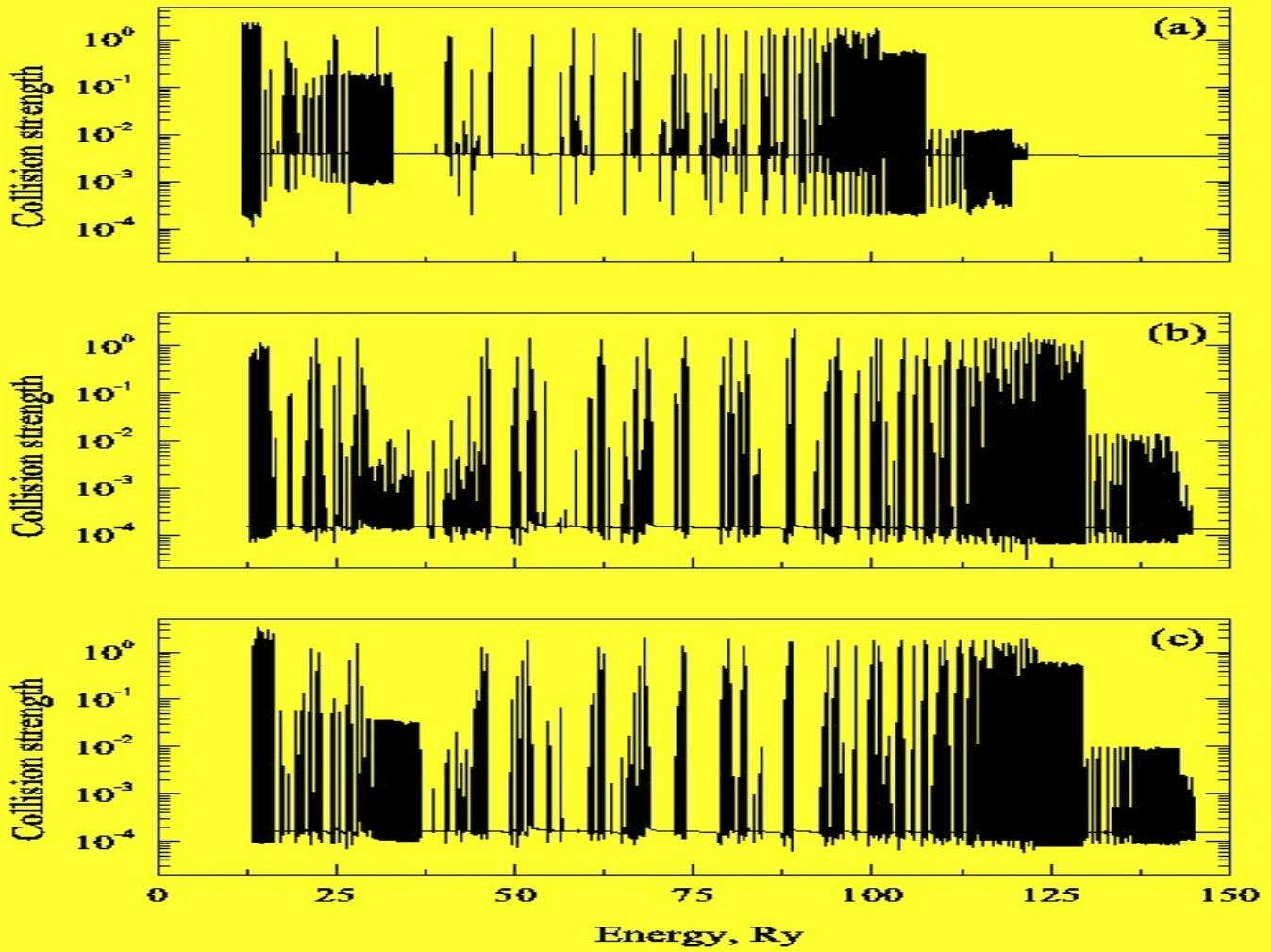
Electron-impact excitation C^{2+}



Electron-impact excitation Fe^{22+}



Electron-impact excitation W^{70+}



Outlook

General form of QRHF equations

$$\left\{\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}-V(nl|r)-\varepsilon_{nl}\right\}P(nl|r)-X(nl|r)+\ non-relativistic\ terms$$

$$\frac{\alpha^2}{4}\left(\varepsilon_{nl}+V(nl|r)\right)^2 P(nl|r)+\frac{\alpha^2}{4}\left(\varepsilon_{nl}+V(nl|r)\right)X(nl|r)+\ mass-velocity\ terms$$

$$\frac{\alpha^2}{4}\left(\delta_{l,0}+\frac{1}{3}\delta_{l,1}\right)\frac{\frac{dU(r)}{dr}\left(\frac{d}{dr}-\frac{1}{r}\left(\alpha^2 Z^2\delta_{l,1}\left(-\frac{37}{30}-\frac{5}{9n}+\frac{2}{3n^2}\right)+1\right)\right)P(nl|r)}{1-\frac{\alpha^2}{4}\left(\varepsilon_{nl}+V(nl|r)\right)}=0\ \ contact\ term$$

Main Distinctions

- No statistical potentials are used. Only conventional self-consistent filed direct $V(nl|r)$ and exchange $X(nl|r)$ potentials in **QRHF**
- The finite size of nucleus is considered determining potential $U(r)$
- The mass-velocity term splits into two parts
- No two-electron potentials in the numerator
- Only direct part of $V(nl|r)$ in denominator of the contact interaction
- Contact interaction woth nucleus is defined both for s-electrons and p-electrons

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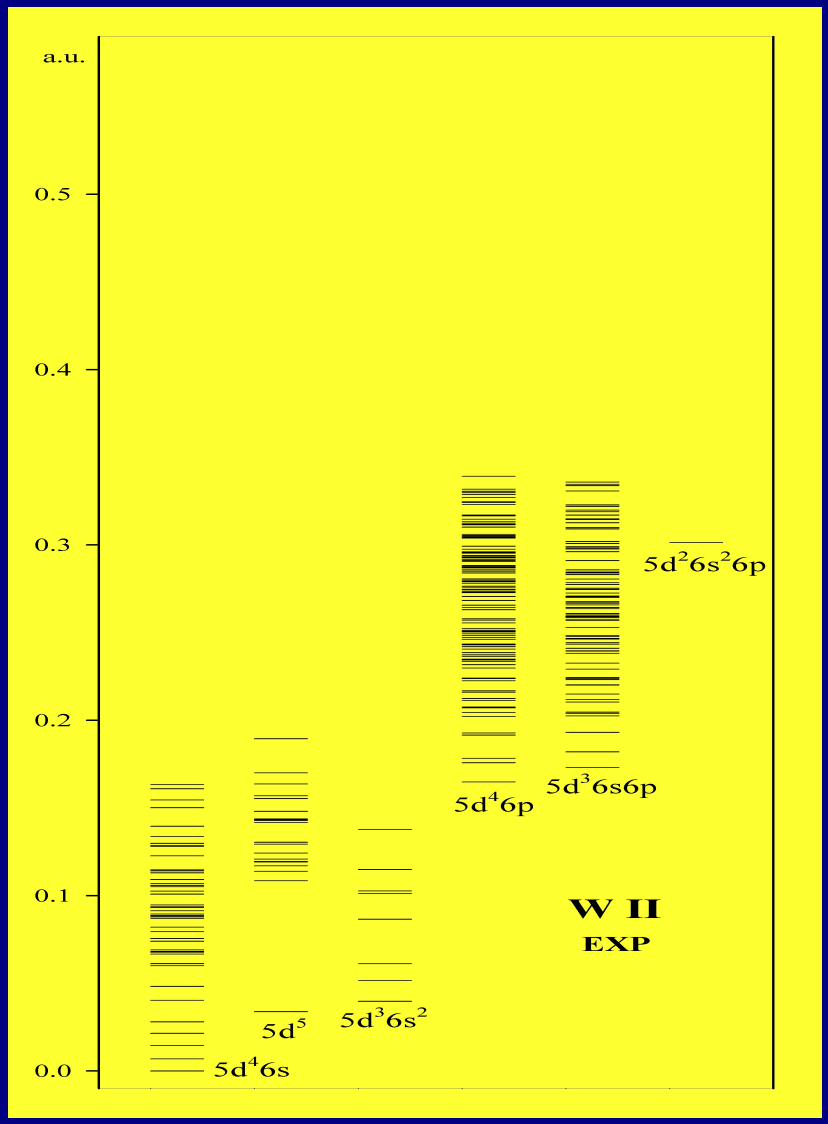
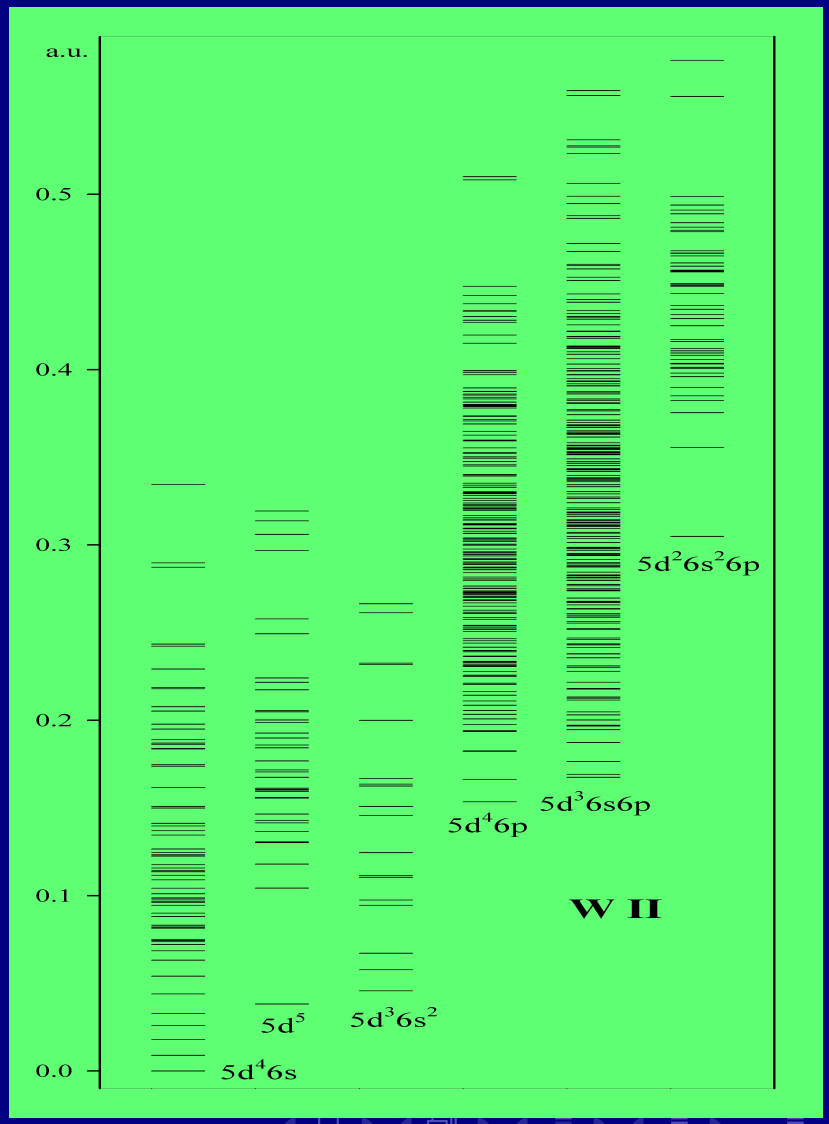
Energy Levels for W II





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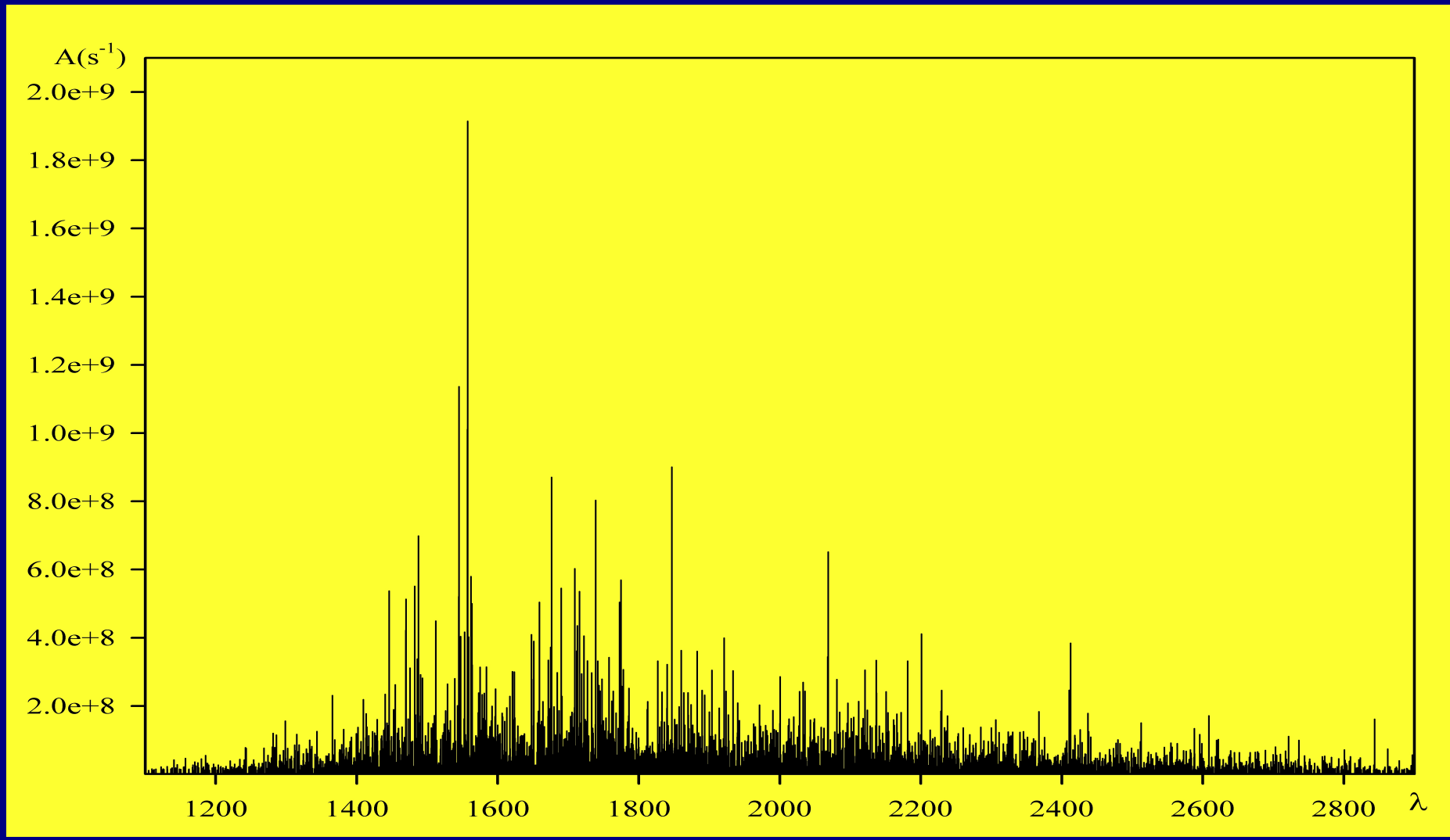
Transition probabilities for W II



Summary

- Method of Relativistic Integral Analogues (ARI) for electron scattering calculation
- Quasirelativistic Hartree-Fock (QRHF) approach for discete spectra

Acknowledgments

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- P. Bogdanovich
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