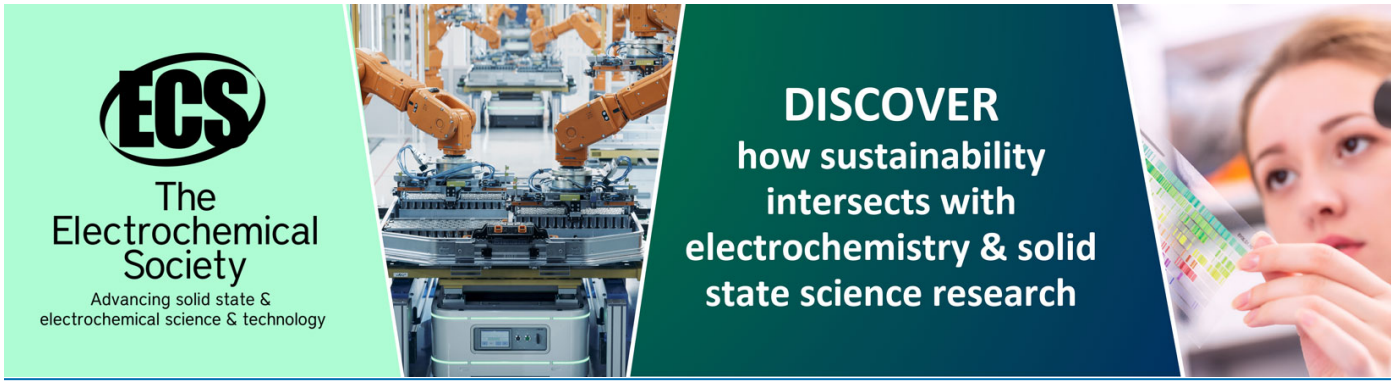
# Benchmark calculations for photoionization of neutral iron





# Benchmark calculations for photoionization of neutral iron

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**Synopsis** The B-spline R-matrix method is used to investigate the photoionization of neutral iron from its ground and the lowest 43 excited states in the energy region from the ionization thresholds to 2 Ry. The sensitivity of the predictions is checked by comparing results obtained in different approximations. Including all terms from the $3d^64p$ and $3d^54s4p$ configurations considerably changes both the low-energy resonance structure and the background cross sections.

The enormous importance of iron-peak elements for astronomical observations is well known. Reliable photoionization cross sections for neutral iron, for example, are a requirement for accurate chemical abundances in late-type stars. The cross sections for ionization processes from both the ground and low-lying excited states are usually the minimum requirement for detailed nonlocal thermodynamic equilibrium modeling. Over several decades, calculations of photoionization cross sections for Fe I were carried out in a variety of approximations, with increasing size and sophistication. Presently, however, both electron-impact excitation rates and photoionization cross sections for Fe still represent a significant source of uncertainty in the models.

The purpose of the present work is to perform more elaborate and extensive calculations for photoionization of Fe I than what is currently available and, thereby, check the convergence of the predicted cross sections. Our improvements include both principal aspects of the collision calculations, namely the accuracy of the target states and the size of the close-coupling expansion.

The calculations were carried out with the B-spline R-matrix (BSR) code [1], where a B-spline basis is employed to represent the one-electron orbitals. Within this method, nonorthogonal sets of term-dependent orbitals are extensively used in both the target description and the representation of the scattering functions. That, in connection with multiconfiguration target expansions, provides a systematic way to account for a variety of correlation and relaxation effects. This feature was illustrated in detail in our recent calculations for electron collisions with Fe I [2] and Fe II [3], where the flexibility of the code allowed us to generate a target description of unprecedented accuracy for collision calculations.

The present close-coupling expansion contains all terms of the $3d^64s$, $3d^54s^2$, $3d^7$, $3d^64p$, and $3d^54s4p$ configurations of Fe II. This set of final target states covers all major channels in photo-ionization of neutral iron and thus provides a basis for approaching convergence in the predicted cross sections. The present photoionization cross sections exhibit significant differences compared to earlier results, in particular with the most recent R-matrix calculations of Bautista *et al.* [4]. We argue what none of the previous calculations can be considered converged due to the omissions of important states in the residual-ion expansions. For example, photoionization of the $3d^64s4p$ states of Fe I can occur in the one-electron approximation through ionization of the 3d, 4s, or 4p electron, respectively, thus leading to the $3d^54s4p$, $3d^64p$, and $3d^64s$ final ionic states of Fe II. To obtain converged results, all these channels should be considered on equal footing. In particular, we found that 3d-ionization becomes the dominant channel for higher energies. This leads to approximately the same value (~10 Mb) of the photoionization cross sections for all Fe I states.

We obtained total and partial photoionization cross sections for the first 44 bound states of Fe I. The photoionization of neutral iron exhibits numerous scattering channels. We performed a detailed analysis of these channels, showing that the relative population of the different ionic states changes considerably when varying the photon energy.

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## References

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