Abstract Submitted
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Benchmark calculations for photoionization of neutral iron from the ground and excited states.[1] OLEG ZATSARINNY, KLAUS BARTSCHAT, Drake University, LUIS FERNANDEZ-MENCHERO, Queen's University Belfast, SWARAJ S. TAYAL, Clark Atlanta University — The B-spline R-matrix method [1,2] is used to investigate the photoionization of neutral iron from the ground and excited states in the energy region from the ionization thresholds to 2 Ry. The multi-configuration Hartree-Fock method in connection with adjustable configuration expansions and term-dependent orbitals is employed for an accurate representation of the initial states of Fe I and the target wave functions of Fe II. The close-coupling expansion contains 261 LS states of Fe II and includes all levels of the $3d^6 4s$, $3d^5 4s^2$, $3d^7$, $3d^6 4p$, and $3d^5 4s 4p$ configurations. Full inclusion of all terms from the principal configurations considerably changes both the low-energy resonance structure and the energy dependence of the background cross sections. Partial cross sections are analyzed in detail to clarify the most important scattering channels. Comparison with other recent calculations such as [3] is used to place uncertainty bounds on the predicted photoionization cross sections and to assess the likely uncertainties in the existing data sets. [1] O. Zatsarinny, Comp. Phys. Comm. **174** (2006) 273. [2] O. Zatsarinny and K. Bartschat, J. Phys. B **46** (2013) 112001. [3] M. A. Bautista, K. Lind, and M. Bergemann, A & A **606** (2017) A127. (2017).

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