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B-Spline Breit-Pauli R-matrix calculations for electron collisions with Krypton and Xenon.¹ KLAUS BARTSCHAT, OLEG ZATSARINNY, Drake University — We have extended our previous work on electron collisions with Ne [1] and Ar [2] to the heavier noble gas targets Kr and Xe. In our *B*-Spline *R*-matrix method [3,4], relativistic effects are accounted for through the most important terms of the Breit-Pauli hamiltonian in the inner region of the *R*-matrix box. Several sets of non-orthogonal valence orbitals were employed to account for the strong term dependence in the one-electron orbitals. Using non-orthogonal basis sets avoids the need for pseudo-orbitals to improve upon the target description and virtually eliminates pseudo-resonance problems. The agreement between our predictions and experiment [5] is much better than obtained in previous calculations based on the standard *R*-matrix approach with strictly orthogonal orbitals, particularly in details such as resonance positions and widths. Consequently, the new results are expected to represent a significant improvement of the current database for electron collisions with heavy noble gases.

[1] O. Zatsarinny and K. Bartschat, J. Phys. B **37** (2004) 2173.

[2] O. Zatsarinny and K. Bartschat, J. Phys. B 37 (2004) 4693.

[3] O. Zatsarinny and C. Froese Fischer, J. Phys. B 33 (2000) 313.

[4] O. Zatsarinny, Comp. Phys. Commun. 174 (2006) 274.

[5] S.J. Buckman and C.W. Clark, Rev. Mod. Phys. 66 (1994) 539.

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