Abstract Submitted for the GEC16 Meeting of The American Physical Society

Electron-impact excitation and ionization of boron. KEDONG WANG, Henan Normal University, OLEG ZATSARINNY, KLAUS BARTSCHAT, Drake University — We present a comprehensive study of electron collisions with neutral boron atoms [1]. The calculations were performed with the B-Spline R-matrix (close-coupling) method [2], by employing a parallelized version of the associated computer code [3]. Elastic, momentum-transfer, excitation, and ionization cross sections were obtained for all transitions involving the lowest 11 states of boron, for incident electron energies ranging from threshold to 100 eV. A multiconfiguration Hartree-Fock method with non-orthogonal term-dependent orbitals was used to generate accurate wavefunctions for the target states. Close-coupling expansions including 13, 51, and 999 physical and pseudo-states were set up to check the sensitivity of the predictions to variations in the theoretical model. The cross-section dataset generated in this work is expected to be the most accurate one available today and should be sufficiently comprehensive for most modeling applications involving neutral boron.

- K. Wang, O. Zatsarinny, and K. Bartschat, Phys. Rev. A 93 (2016) 052715.
- [2] O. Zatsarinny and K. Bartschat, J. Phys. B 46 (2013) 112001.
- [3] O. Zatsarinny, Comp. Phys. Commun. 174 (2006) 273.

¹Work supported by the China Scholarship Council and the United States National Science Foundation under grants PHY-1403245 and PHY-1520970, and by the XSEDE allocation PHY-090031.

Klaus Bartschat Drake University

Date submitted: 08 Jun 2016 Electronic form version 1.4