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Calculation of inner-shell photoionization of ground state Na: relativistic vs. nonrelativistic calculation H.-L. ZHOU, S.T. MANSON, Georgia State University, A. HIBBERT, Queen's University of Belfast — Calculations of inner-shell photoionization of ground state Na over the photon energy range 40-100 eV have been performed using nonrelativistic LS coupling and relativistic Breit-Pauli (BP) R-matrix approximations. The BP R-matrix calculation adds the spin-orbit, mass-correction and Darwin terms to the non-relativistic Hamiltonian in order to include relativistic effects, giving 111 J-dependent states of Na+ from 61 LS states; the same target orbitals are used for both calculations. The calculated energy of ground state of Na is 5.1606 eV in LS coupling and 5.1756 eV in BP approximation (NIST value is 5.14 eV). We find that in the neighborhood of the broad $2s\rightarrow np$ resonances, the results of LS and BP calculations are almost same, but in the neighborhood of narrow doubly-excited $2p^5 nln'l'$ resonances, the BP calculations show spin-orbit splittings and differ significantly from the LS coupling results.

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