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charge krypton ions

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(Submitted on 19 Jul 2011)

We present multi-configuration Breit-Pauli distorted-wave photoionization (PI) cross sections and radiative recombination (RR) and dielectronic recombination (DR) rate coefficients for the first six krypton ions. These were calculated with the AUTOSTRUCTURE code, using semi-relativistic radial wavefunctions in intermediate coupling. Kr has been detected in several planetary nebulae (PNe) and H II regions, and is a useful tracer of neutroncapture nucleosynthesis. PI, RR, and DR data are required to accurately correct for unobserved Kr ions in ionized nebulae, and hence to determine elemental Kr abundances. PI cross sections have been determined for ground configuration states of Kr^0--Kr^5+ up to 100 Rydbergs. Our Kr^+ PI calculations were significantly improved through comparison with experimental measurements. RR and DR rate coefficients were determined from the direct and resonant PI cross sections at temperatures (10^1--10^7)z^2 K, where z is the charge. We account for Delta n=0 DR core excitations, and find that DR is the dominant recombination mechanism for all but Kr^+ at photoionized plasma temperatures. Internal uncertainties are estimated by comparing results computed with three different configuration-interaction expansions for each ion, and by testing the sensitivity to variations in the orbital radial scaling parameters. The PI cross sections are generally uncertain by 30-50% near the ground state thresholds. Near 10⁴ K, the RR rate coefficients are typically uncertain by <10%, while those of DR exhibit uncertainties of factors of 2 to 3, due to the unknown energies of near-threshold autoionizing resonances. With the charge transfer rate coefficients presented in the third paper of this series, these data enable robust Kr abundance determinations in photoionized nebulae for the first time.

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