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Electron scattering from krypton: High-resolution electron scattering experiments and B-spline R-matrix calculations

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Synopsis For elastic scattering and electron impact excitation of the $4p^5 5s$ states in Kr, we present independently normalized, absolute angle-differential cross sections over the entire angular range ($0^\circ - 180^\circ$). Excellent agreement is obtained between the present experimental data and theoretical predictions from a fully relativistic B-spline R-matrix (close-coupling) model.

In a joint experimental and theoretical effort, we carried out a detailed study of elastic scattering and electron impact excitation of the $4p^5 5s$ states in Kr. The incident electron energy resolution was about 13 meV at a current of about 400 pA. A specially designed magnetic angle changer allowed for measurements up to 180° scattering angle.

The calculations were performed in a fully relativistic Dirac B-spline R-matrix (DBSR) framework [1]. To resolve the wealth of near-threshold resonance structure in the electron-impact excitation process, we coupled 69 states with principal configurations $4p^6$, $4p^5 5s$, $4p^5 5p$, $4p^5 4d$, $4p^5 6s$, $4p^5 7s$, $4p^5 6p$, $4p^5 4d$, and $4p^5 4f$, respectively. The valence spinors were generated through a B-spline bound-state close-coupling calculation using a number of Kr^+ states with frozen core orbitals. The latter also included states with only one electron in the 4s orbital. Hence this DBSR69 model included the most important core-valence correlations in an *ab initio* manner.

To describe elastic scattering below the first excitation threshold, we used a DBSR_pol model that only included the $4s^2 4p^6$ ground state with total electronic angular momentum $J = 0$ and a single pseudostate $|\psi_p\rangle$ with $J = 1$ constructed from the configurations $4s^2 4p^5 \bar{5}s$, $4s^2 4p^5 \bar{4}d$, and $4s 4p^6 \bar{5}p$, respectively. The polarized pseudostate allows for a very accurate description of low-energy elastic scattering, based on first principles without using semiempirical polarization potentials. Our pseudostate yielded a dipole polarizability of 17.3 a_0^3, in excellent agreement with the recommended value of 17.075 a_0^3 [4].

As seen in the figure, our present experimental data clearly improve the agreement between experiment and theory relative to our earlier comparison [2] with the data of Phillips [3].

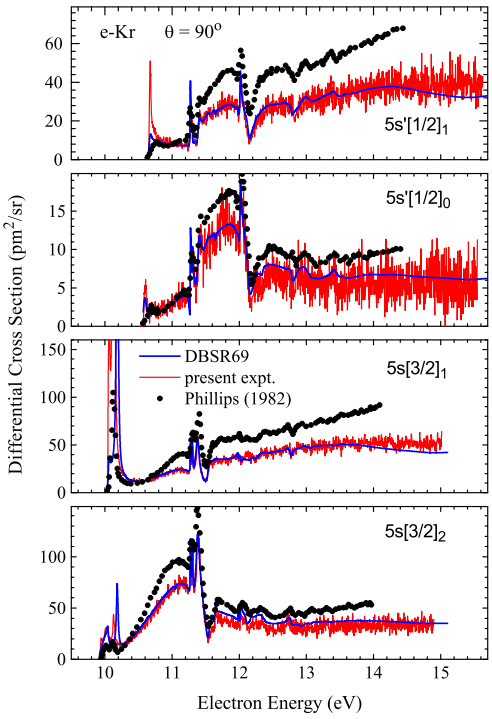

Figure 1. Differential cross section for electron-impact excitation of Kr at a scattering angle of 90°.

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