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Observing K-shell pre-edge resonances in Kr, Xe, and XeF₂¹
STEPHEN SOUTHWORTH, ROBERT DUNFORD, ELLIOT KANTER, GILLES DOUMY, PHAY HO, ANNE MARIE MARCH, LINDA YOUNG, Argonne National Laboratory, LAN CHENG, Johns Hopkins University — Rydberg transitions below the K-shell ionization thresholds of Kr and Xe are obscured in x-ray absorption spectra due to core-hole lifetime broadening. However, excitation of these resonances produce spectator electrons as the core holes decay by radiative and radiationless transitions. We report on ion charge-state distributions of Kr and Xe in coincidence with x-ray fluorescence as the absorbed x-ray energy is scanned through pre-edge resonances and ionization thresholds. Shifts of ion yields from higher to lower charge states are observed in the resonance regions that we attribute to spectator electrons. In XeF₂, the F ligands modify the valence electron charge distribution, resulting in a chemical shift of the Xe 1s ionization energy. Strong excitation of the lowest unoccupied molecular orbital (LUMO) is also observed and modifies the ion spectra due to molecular alignment. The measured LUMO and ionization energies are compared with relativistic coupled-cluster calculations that treat relativistic and electron correlation interactions on the same footing.

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