

Abstract Submitted  
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**Observation of  $K$ -shell resonances in Xe and XeF<sub>2</sub>**<sup>1</sup> STEVE SOUTHWORTH, ROBERT DUNFORD, DIPANWITA RAY, ELLIOT KANTER, BERTOLD KRÄSSIG, LINDA YOUNG, DON WALKO, Argonne National Laboratory — We recently reported on the ion charge states and fragmentation channels of Xe and XeF<sub>2</sub> following  $K$ -shell x-ray absorption by the Xe atom [1]. The ion spectra reveal effects of resonant excitations despite the 11.49-eV lifetime width of the vacancy states. Due to the high electronegativity of the F ligands, Xe forms stable molecules such as XeF<sub>2</sub>. With 10 valence electrons, XeF<sub>2</sub> is a prime example of a hypervalent molecule and its structure has attracted interest since its discovery in the 1960s. A strong pre-edge resonance is observed in the x-ray absorption spectrum that we attribute to the antibonding  $7\sigma_u$  orbital. Excitation of the  $7\sigma_u$  resonance selects a spatially aligned ensemble of molecules as observed in our ion fragmentation spectra [1]. Analysis of the x-ray absorption spectrum also yields a measurement of the chemical shift of the Xe 1s ionization energy resulting from the F ligands. Results of new measurements on Xe and XeF<sub>2</sub> with an improved x-ray/ion coincidence instrument will also be reported.

[1] R. W. Dunford *et al.*, Phys. Rev. A **86**, 033401 (2012).

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