X-ray absorption spectroscopy study on h-LuFeO$_3$ and h-YbFeO$_3$† XIAOSHAN XU, University of Nebraska-Lincoln, Nebraska Center for Materials and Nanoscience, SHI CAO, TULA PAUDEL, KISHAN SINHA, XUANYUAN JIANG, University of Nebraska-Lincoln, Nebraska Center for Materials and Nanoscience, WENBIN WANG, Fudan University, JIAN WANG, Canadian Light Source, EVGENY TSYMBOL, PETER DOWBEN, University of Nebraska-Lincoln, Nebraska Center for Materials and Nanoscience — We have studied the unoccupied electronic band structure of the hexagonal ferrites h-LuFeO$_3$ and h-YbFeO$_3$ using the absorption spectroscopy obtained with linearly polarized soft X-ray synchrotron radiation. The shapes of the spectra have been analyzed in terms of the splitting of atomic energy levels in various crystal fields corresponding to the local symmetry of the different atomic sites. Significant hybridization between O-2p and various iron and rare earth orbitals (such as Fe-3d, Lu/Yb-5d and Yb-4f) have been observed. The spectral weight contributions to the electronic states near the bottom of the conduction band are found to consist of Fe-3d, Lu/Yb-5d, and Yb-4f as relatively narrow bands, as well as a wide O-2p band covering much of the measured energy range. The results are consistent with the density functional theory calculation including onsite-Coulomb repulsion corrections in terms of Hubbard U.

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