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Site Sensitivity and local electronic symmetries in carboranes T.T. FISTER, G.T. SEIDLER, F.D. VILA, University of Washington, J.O. CROSS, Advanced Photon Source, Argonne National Laboratory, J.C. LINEHAN, Pacific Northwest National Laboratory — Icosohedral carboranes containing ten boron and two carbon atoms are seeing renewed interest because of their potential use in new cancer and AIDS therapies. These molecules have flexible geometries which allow bonding to three types of carbon sites (e.g. *ortho*-, *para*-, and *meta*- configurations). Using a new multielement spectrometer, we present the first x-ray Raman scattering (XRS) study on each isomer with excited state spectra taken from the both the carbon and boron 1s states. The change in the electronic structure between the isomers is most pronounced in the carbon spectrum, where the position in the edge confirms prior density functional theory calculations. With the boron spectra, we used the unique momentum transfer dependence of XRS to extract the symmetry components of the density of unoccupied states, i.e. the l-DOS. These results give an improved picture of the local electronic properties of the carboranes.

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