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Photo-fragmentation of the closo-carboranes JING LIU, DANQIN FENG, P.A. DOWBEN, Dept. of Physics and Astronomy, University of Nebraska-Lincoln, A.P. HITCHCOCK, Dept. of Chemistry, McMaster University, Canada, A.L.D. KILCOYNE, T. TYLISZCZAK, Advanced Light Source, Lawrence-Berkeley Laboratory, J.D. BOZEK, Stanford Synchrotron Radiation Laboratory, E. RÜHL, Institut für Physikalische Chemie, Freie Universität Berlin, Germany — Single and multi-cation ionic fragmentation of three isomeric carborane cage compounds [closo-1,2-orthocarborane, closo-1,7-metacarborane, closo-1,12-paracarborane ($C_2B_{10}H_{12}$)] following B 1s and C 1s excitation were studied by time of flight mass analysis. The energetic cycles were constructed to gain some insights into some of decomposition processes. CH^+ or BH_2^+ fragment dominates the single ion fragmentation of the closo-carboranes. Double ion fragmentation yields and charge separation mass spectra of all three isomers are generally quite similar in that H^+ and BH_2^+/CH^+ ion pairs, BH_2^+/CH^+ and Y_{11}^+ion pairs (where Y = (BH) or (CH)), Y_3^+ and Y_9^+ion pairs (where Y = (BH) or (CH)) yields dominate. The H^+ and BH_2^+/CH^+ ion pairs dominate at the B 1s threshold for ortho- and metacarborane, while Y_1^+ and Y_{11}^+ion pairs (where Y = (BH) or (CH)) dominates the multi-photofragment ion yield of paracarborane at the B1s threshold.

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