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The electronic structure of Co and Ni tetraazaannulenes JING LIU, JIE XIAO, P. JEPPSON, P.A. DOWBEN, Department of Physics and Astronomy, University of Nebraska-Lincoln, SEOK-BONG CHOI, L. JARABEK, A.N. CARUSO, Center for Nanoscale Science and Engineering, North Dakota State University, YA.B. LOSOVYJ, Center for Advanced Microstructures and Devices, Louisiana State University — We compare two metal centered tetraazaannulene (TMTAA) macrocyclic complex molecules: 5,7,12,14- tetramethyl -2,3:9,10- dibenzo [b,i] -1,4,8,11- tetraazacyclotetradecine nickel (II) and 5,7,12,14- tetramethyl -2,3:9,10- dibenzo [b,i] -1,4,8,11- tetraazacyclotetradecine cobalt (II). The highest occupied molecular orbital to the lowest unoccupied molecular orbital gap, obtained from combined ultraviolet photoemission and inverse photoemission studies, is close to the expected value of 6.6 eV expected from simple model calculations. While both the Co(II) (s=1/2) and Ni(II) (s=0) tetramethyldibenzo-tetraazaannulene molecular electronic structures are very similar, the Ni(II) adopts a high symmetry molecular configuration upon adsorption, with a strong preferential orientation. The role of an unpaired electron upon molecular symmetry and stability is discussed.

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