Quantum chemically derived models have gained some acceptance in the past decades, but it still holds that the value of a bonding model is primarily judged by the simplicity of its application, rather than by its theoretical justification. DFT has proven to be very powerful because the Kohn-Sham orbital turned out to be even more helpful for a bonding analysis in terms of orbital interactions than the Hartree-Fock orbital, since the former include correlation effects. Many more complexes with a formal d⁰ configuration of the central metal (and also with d¹ and d² configurations) have since been found, both experimentally and computationally, which do not conform to the simple structural models. In this research the structure and vibrational frequencies of a number of chromium, molybdenum and tungsten complexes optimized and studied by DFT and HF methods used LANL2DZ basis set. The calculations results confirm experimental data such as X-ray single crystal diffractions. All of these data could be explained by sdⁿ hybridation and non-VSEPR structural model.