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Electron Counting *vs* Geometry in transition metal complexes

Electron counting is a powerfull tool to rationalize the geometry of most of transition metal complexes. The family of ML_4 complexes is a well known example with a square-planar structure for d^8-diamagnetic complexes and a tetrahedral geometry for the d^{10} complexes. However these simple relationships between the number of d electrons and the shape of the ML_n molecule no longer apply with strong π acceptor ligands such as biphosphinine (the P analog of bipyridine). This point is illustrated by DFT caculations on complexes d^{10}-$M(L\text{-}L)_2^q$ (L-L = biphosphinine (bp); M = Ru, Co Rh, Ni, Pt) and d^6-$M(L\text{-}L)_3^q$ (L-L = biphosphinine (bp), bipyridine (bpy); M = Ti, Zr, Hf, Mo, W, Ru) which have been synthetized for the most in our laboratory. DFT calculations followed by a molecular orbital analysis allow a rationalization of the unexpected geometry found for the complexes with bp ligands .

Interactions

Theory ⟺ experiments