Synthesis and Structural Analysis of a Number of Hexacoordinate Heteroleptic Non-VSEPR Molybdenum and Tungsten Complexes

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The development of improved models for chemical bonding has always benefited from specific cases in which the existing models fail. One well-known example is the failure of the widely used Valence Shell Electron Pair Repulsion (VSEPR) model. In recent years, many exceptions, represented by "Non-VSEPR" compounds, have been reported. On the basis of ligands similarity these compounds are classified as "homoleptic" and "heteroleptic" systems. Because of their simplicity, homoleptic systems have been studied more than heteroleptic systems. [1], [2] Many quantum chemical calculations on these systems have have been reported in the past years. Tungsten and molybdenum complexes have an important role in the extention of non–VSEPR structures and bonding in d^0 systems.[3] In this research a number of hexacoordinate heteroleptic complexes of molybdenum and tungsten have been synthesized. Indeed, the distortions from the regular octahedron in heteroleptic hexacoordinate d^0 complexes have played an important historical role in drawing the attention of theoreticians to possible deviations from the usual structures. The structures of these complexes have been characterized by X-ray single crystal diffraction techniques. Experimental data confirm the results of DFT calculations and show good relationship with the Non-VSEPR compounds.

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