Spin State and Stereochemistry in Tetracoordinate Complexes of d^n Transition Metals

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We will present a theoretical study of the structural preferences of tetracoordinate transition metal compounds with d^n electronic configuration. The structural choice of tetracoordinate transition metal compounds has been established recently from the available experimental structural data with the help of the Continuous Shape Measures (CShM)[1] metodology. In that work, different structural preferences were found for the tetracoordinate transition metal compounds as a function of the electron configuration of the metal[3].

Using the Densitity Functional Theory with the B3LYP hybrid functional we have calculated the potential energy surfaces for simple $[M(CH_3)_4]$ models in different spin states of all the d^n electron configurations. By using the CShM methodology we analyze the distribution of more than 12000 structures along the minimal distortion pathway[2] for the tetrahedron to square interconversion, and find that it mirrors the calculated potential energy curves for each d^n family of complexes.

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