

Porphyrins are an important class of biomolecules, which are heavily studied, both experimentally and computationally. But, despite the intensive efforts, for many questions we still aren't able to consistently find an agreement between theory and experiment. One of the still unresolved issues is the character of the ground state of the Fe(II)-porphyrin molecule. We used a model of the Fe(II)-porphyrin molecule to study the effects of geometrical changes on the spin states. By carrying out extensive DMRG-CASSCF calculations topped with TCCSD correlation treatment we are able to link the effects of these geometrical changes to the experimental results, and predict a quintet ground state for the isolated Fe(II)-porphyrin molecule. Also, using a ligated porphyrin belonging to the iron porphyrin carbene class of molecules, we demonstrate by combining the CASSCF and AC0 methods that geometrical changes outside the porphyrin core cannot be overlooked.