



Optimized geometries of representative examples of the metalloporphyrin dimers containing only 5-coordinate, mixed 5- and 6-coordinate and 6-coordinate metal sites. The minimal steric strain of the unligated dimer contributes to its very high dissociative stability despite energetically unfavorable (high) spin of such 5-coordinate Fe(II) or Co(II) sites. Structures were optimized at the B3LYP/6-31G* level of DFT.