Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Materials for: Knockout driven fragmentation of porphyrins

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Dissociation Energies for protonated Tetraphenylporhyrin (TPP+H)

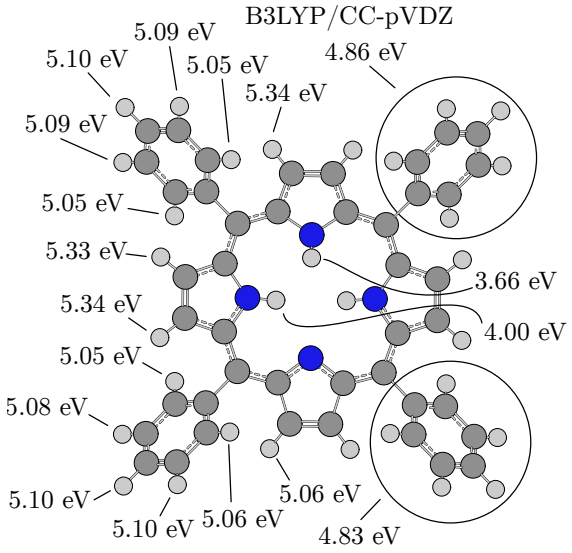

Figure S 1: Dissociation energies for the phenyl groups and different hydrogen positions for protonated Tetraphenylporphyrin $(TPP + H)^+$ molecule, calculated by using Density Function Theory (DFT) at the B3LYP/CC-pVDZ level of theory.

Dissociation Energies for Tetraphenylporhyrin iron (III) (FeTPP)

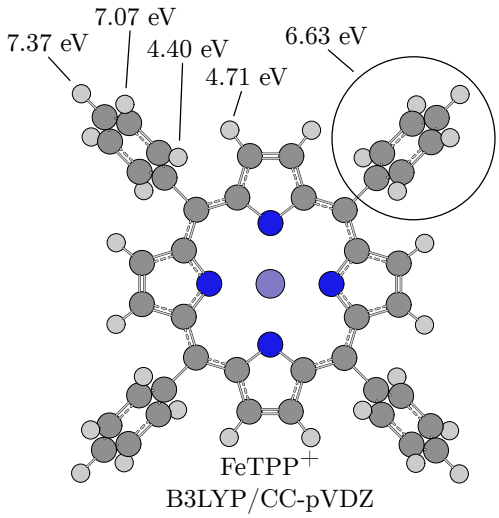

Figure S 2: Dissociation energies for the phenyl groups and different hydrogen positions for Tetraphenylporhyrin iron (III) (FeTPP) molecule, calculated by using Density Function Theory (DFT) at the B3LYP/CC-pVDZ level of theory.