Spectroscopic Studies of Chloroperoxidase Compound II

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Using a combination of density functional calculations and Mössbauer spectroscopy we have examined chloroperoxidase compound II (CPO-II). The Mössbauer spectrum of CPO-II shows for the first time the presence of two distinct ferryl species. Density functional calculations and a previous EXAFS investigation allow us to assign these intermediates as the protonated and unprotonated forms of CPO-II. We find that CPO-II is ≈70% protonated.