

Supplementary Information

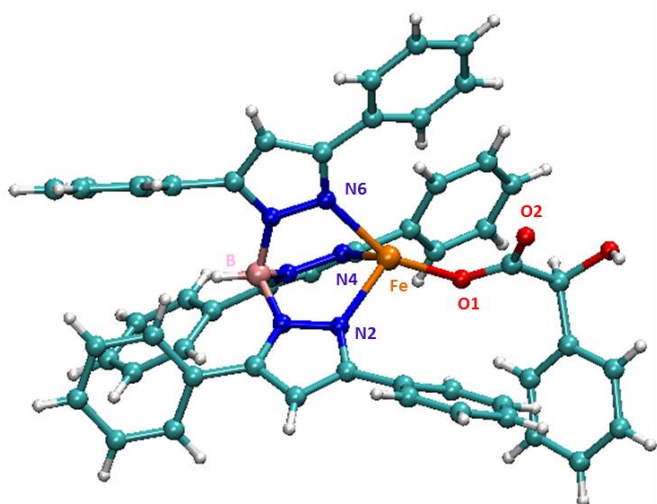
The generation of the oxidant agent of a mononuclear nonheme Fe(II) biomimetic complex by oxidative decarboxylation. A DFT investigation

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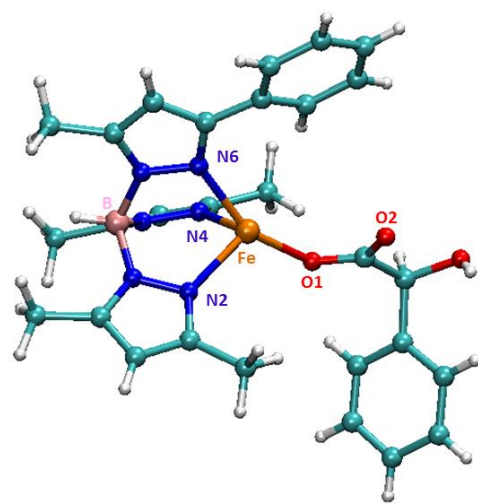
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Table S1. Calculated spin contamination for all investigated complexes under all three spin states co spin states examined.

	3	5	7
a	2.0442	6.0127	12.0233
adduct	3.5769	6.6643	12.0201
TS1	2.0210	6.6945	12.0188
hydroperoxo	2.0294	6.1325	12.0182
TS2	2.0361	6.1380	-
Prod	2.0334	6.0156	12.0297



X-Ray



**Model
(a)**

Figure S1 Crystal structure of hydrotris(3,5-diphenylpyrazole-1-yl)borate) Fe(II)-mandelate and its computational model (a) used in this study.

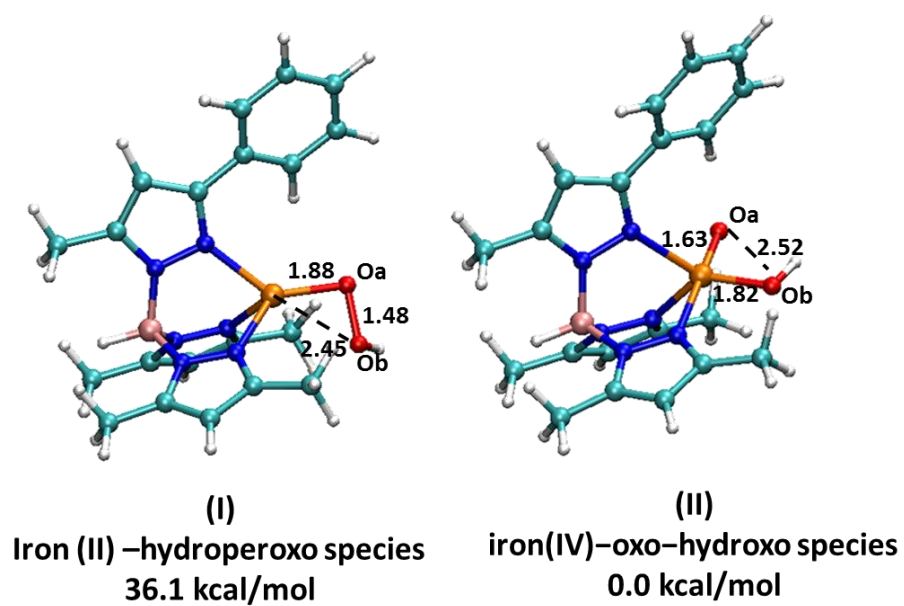


Figure S2 The two possible forms of the product of the oxidative decarboxylation process in quintet species.