

Supplementary information

The Alpha oxygen – the unique oxidation active site from the quantum chemical viewpoint

Stepan Sklenak^a and Jiri Dedecek^{*,a}

^a *J. Heyrovsky Institute of Physical Chemistry of the Czech Academy of Sciences, Dolejskova 3, 18223 Prague, Czech Republic*

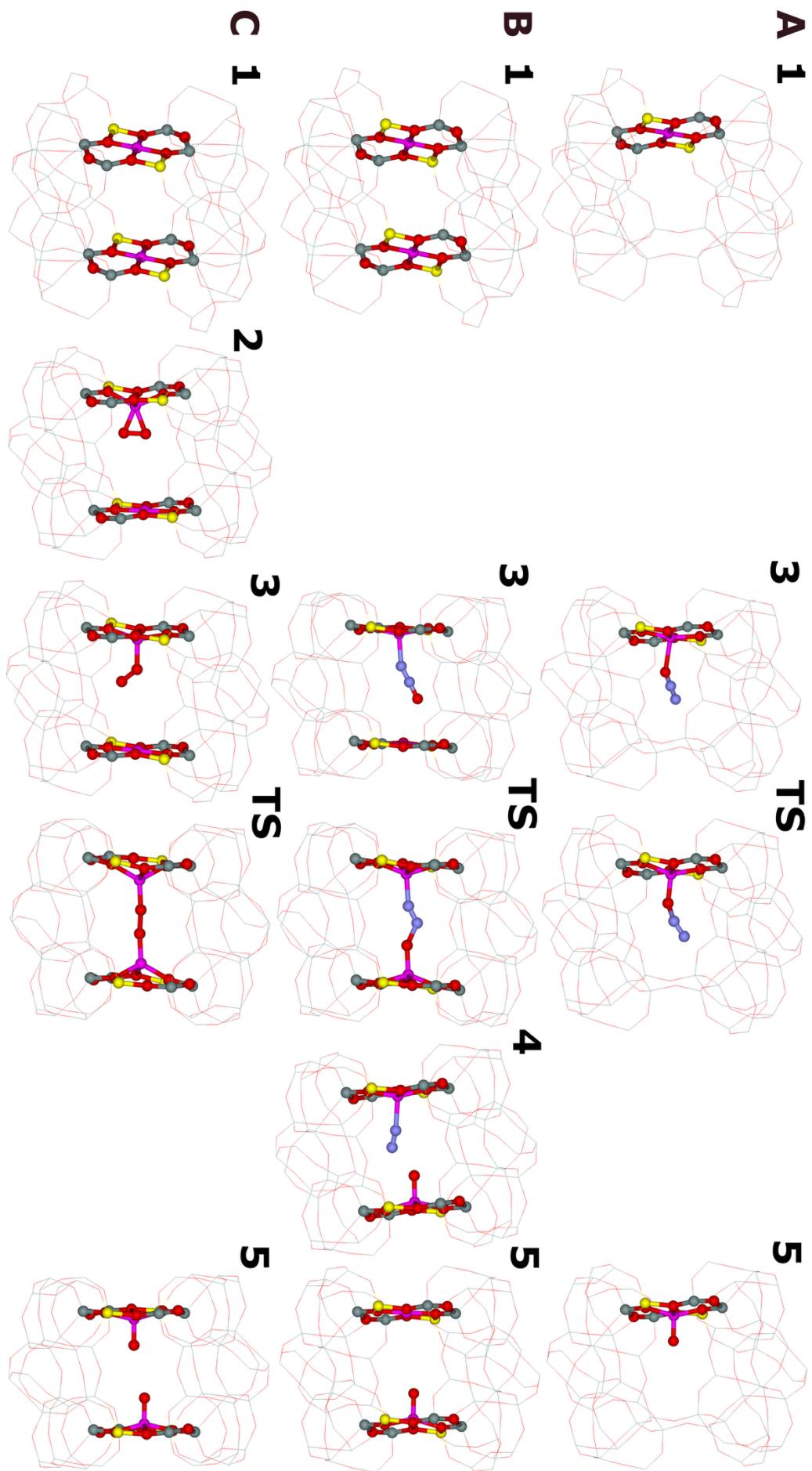


Fig. S1 Optimized structures of all the species involved in the formation of the Alpha oxygen atoms. (A) from N₂O over isolated Fe(II) cations. (B) from N₂O over the distant binuclear Fe(II) cationic sites. (C) from O₂ over the distant binuclear Fe(II) cationic sites. All the Fe cationic sites are $\beta 2$. Silicon atoms are in gray, oxygen atoms in red, aluminum atoms in yellow, nitrogen atoms in blue, and iron atoms in violet.