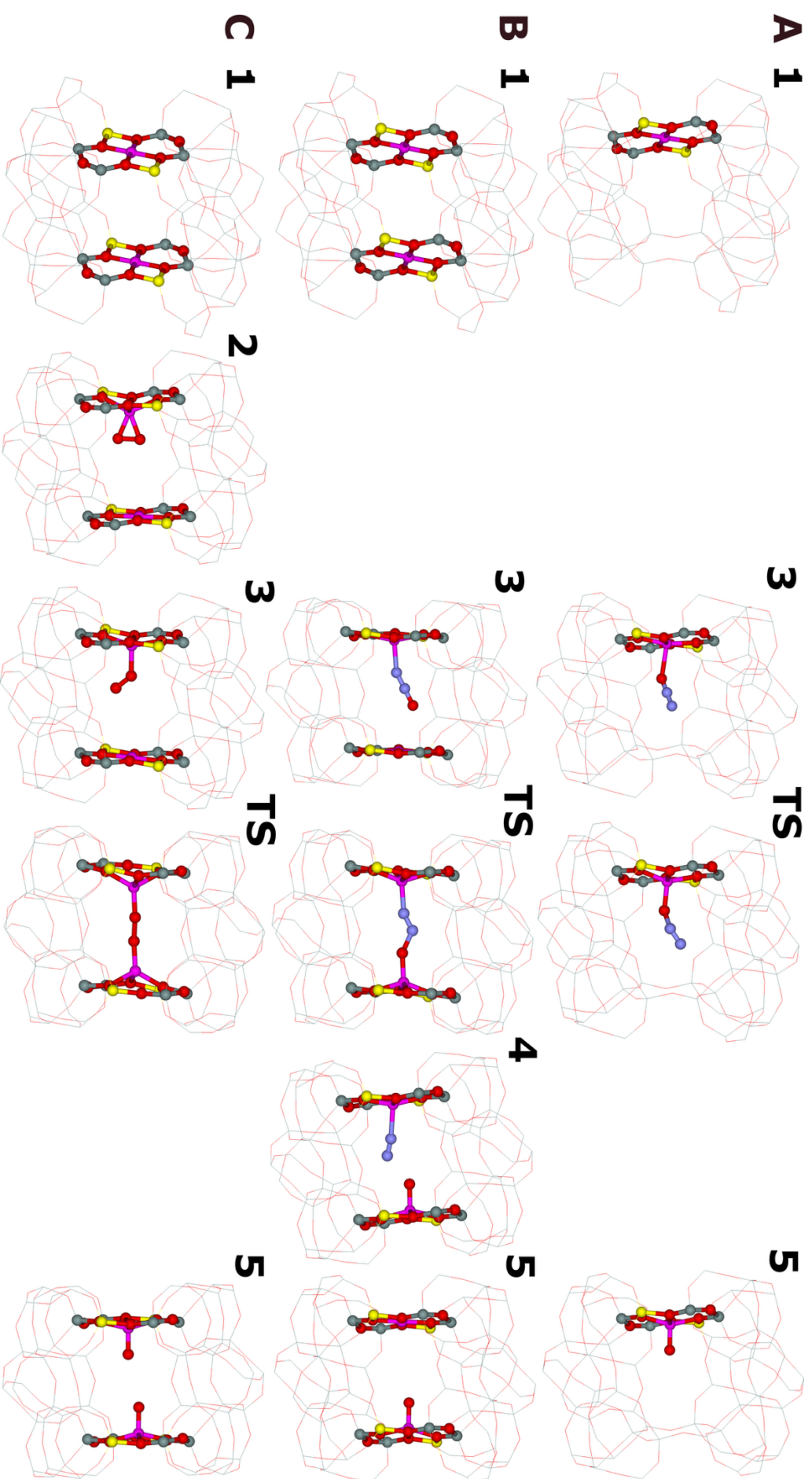


## **Supplementary information**

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

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**Fig. S1** Optimized structures of all the species involved in the formation of the Alpha oxygen atoms. (A) from N<sub>2</sub>O over isolated Fe(II) cations. (B) from N<sub>2</sub>O over the distant binuclear Fe(II) cationic sites. (C) from O<sub>2</sub> 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.