

## SUPPORTING INFORMATION

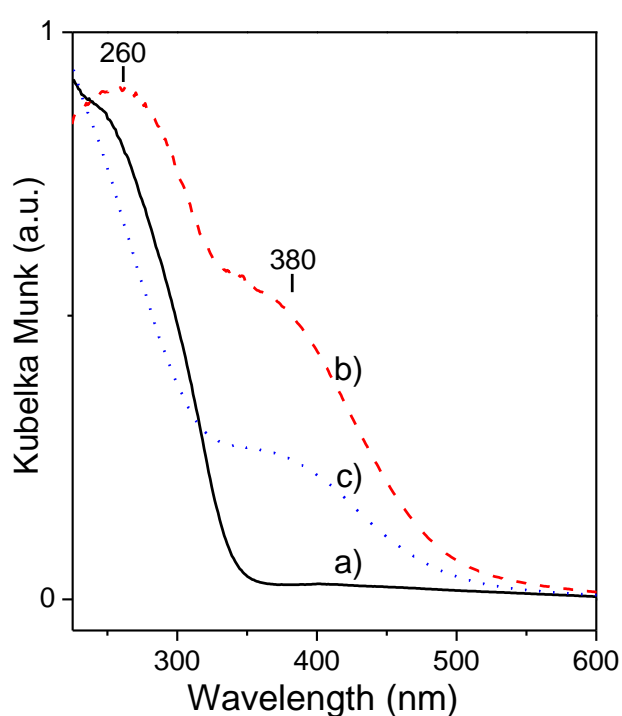
### The Interaction of H<sub>2</sub>O<sub>2</sub> with TiAlPO-5 Molecular Sieves. Probing the Catalytic Potential of Framework Substituted Ti Ions.

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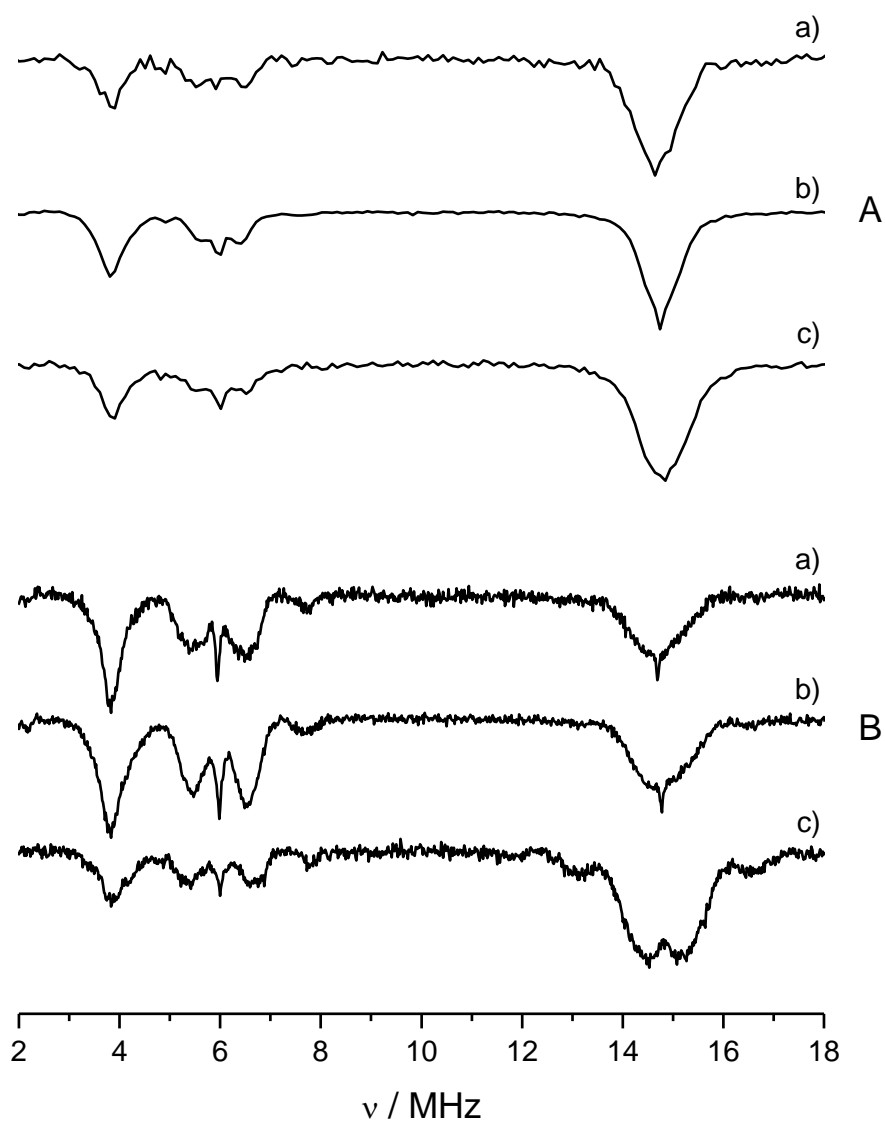
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#### S1 UV-Vis spectra of calcined TiAlPO-5 reacted with aqueous H<sub>2</sub>O<sub>2</sub>.



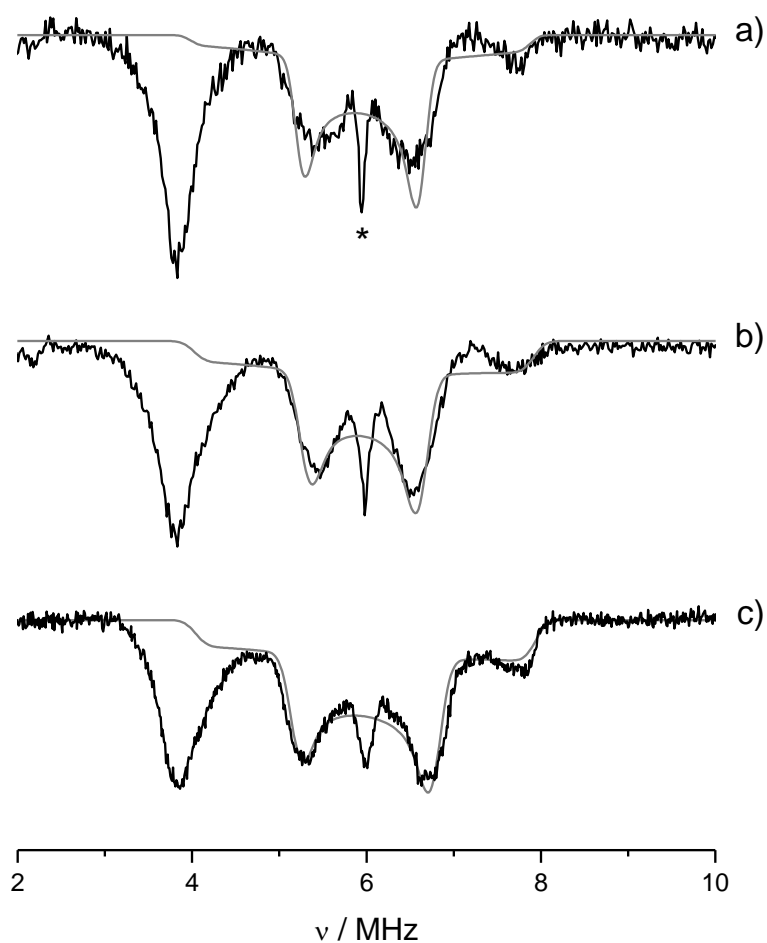
**Figure S1.** DR UV-Vis spectra of a) Calcined TiAlPO-5, b) in contact with aqueous H<sub>2</sub>O<sub>2</sub> and c) after room temperature outgassing. Spectra were arbitrarily normalized for easier comparison.

## S2. Experimental ENDOR Spectra



**Figure S2.** Experimental Mims ENDOR spectra of  $\text{O}_2^-$  on TiAlPO-5 obtained by reaction of the calcined sample with A) hydrated  $\text{H}_2\text{O}_2$  and B) anhydrous  $\text{H}_2\text{O}_2$  (from UHP). The spectra are taken at three different magnetic field settings corresponding to a)  $g_{zz}$  component ( $B_0 = 344.4$  mT), b)  $g_{yy}$  component ( $B_0 = 346.6$  mT) and c)  $g_{xx}$  component ( $B_0 = 348.3$  mT).

### S3. Computer simulations of $^{31}\text{P}$ ENDOR spectra of TiAlPO-5 obtained by reaction with anhydrous $\text{H}_2\text{O}_2$ (from UHP)



**Figure S3.** Experimental (black line) and simulated (grey line)  $^{31}\text{P}$  Mims ENDOR spectra of  $\text{O}_2^-$  on TiAlPO-5 obtained by reaction of the calcined sample with anhydrous  $\text{H}_2\text{O}_2$  (from UHP) measured at three different magnetic field settings corresponding to a)  $g_{zz}$  component ( $B_0 = 344.4$  mT), b)  $g_{yy}$  component ( $B_0 = 346.6$  mT) and c)  $g_{xx}$  component ( $B_0 = 347.7$  mT). The asterisk indicates the  $^{31}\text{P}$  signal belonging to the remote phosphorous nuclei, which are not taken into account in the simulation. The simulated parameters are listed in Table 1 in the main text.