

Electronic Supplementary Information

Kinetics and Mechanism of the OH-radical and Cl-atom Oxidation of Propylene

Carbonate

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Content Summary

The SI contains i) absorbance-time behavior of propylene carbonate and the main product assigned to acetyl formyl carbonate, ii) a product spectrum from the irradiation of a propylene carbonate/Cl₂ mixture in nitrogen (Fig. S2), iii) a concentration-time profile of the identified products from irradiation of a propylene carbonate/Cl₂ mixture in nitrogen (Fig. S3), vi) dependence of the acetic acid yield on oxygen (Fig. S4) and iv) postulated mechanism for acetic acid formation (Scheme S1).

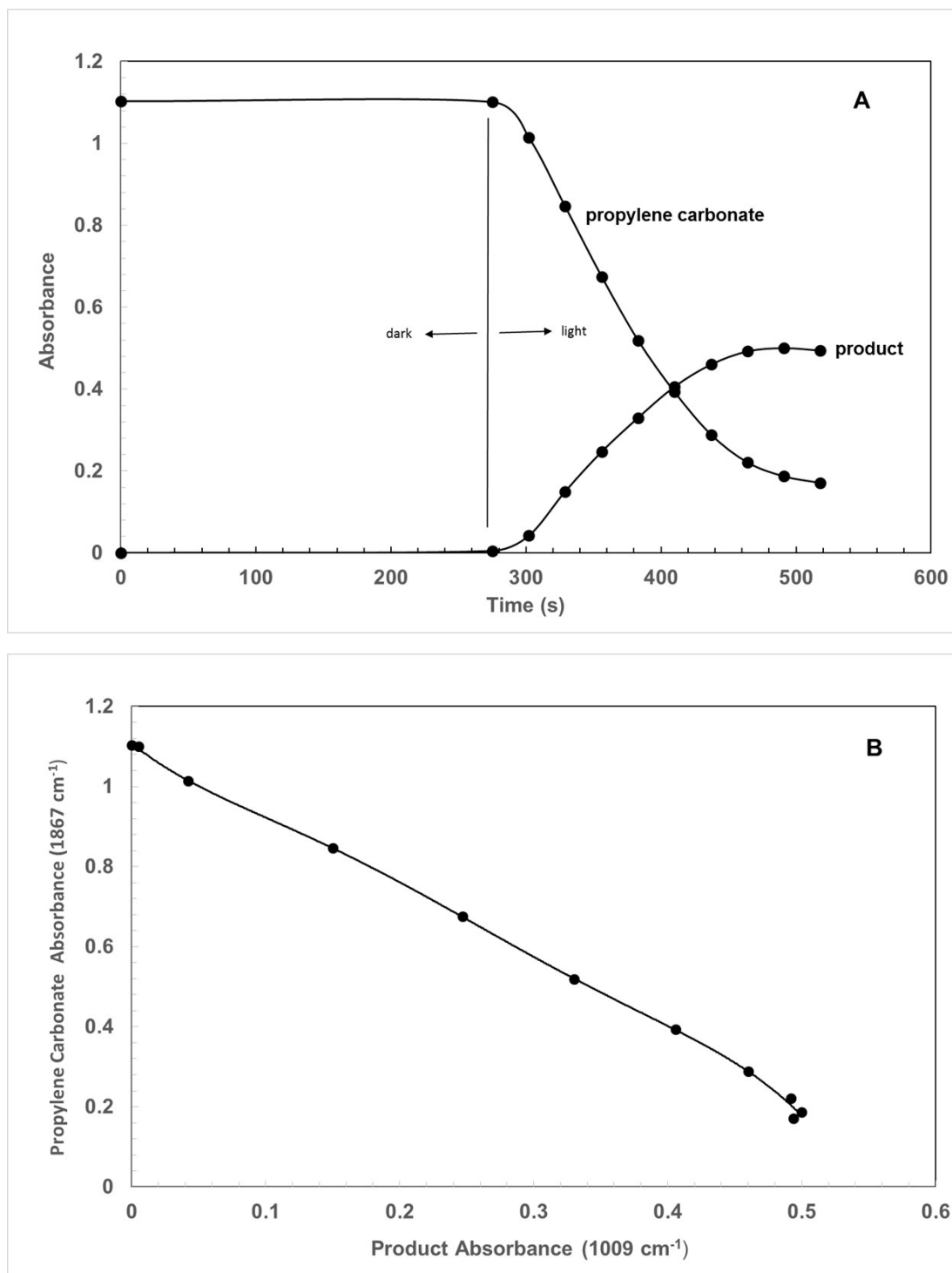


Fig. S1 Panel A shows the absorbance of the carbonyl absorption of propylene carbonate at 1867 cm^{-1} and the absorption of the assigned product acetyl formyl carbonate at 1009 cm^{-1} as a function of time. Panel B shows a plot of the propylene carbonate absorbance at 1867 cm^{-1} versus the product absorbance at 1009 cm^{-1} .

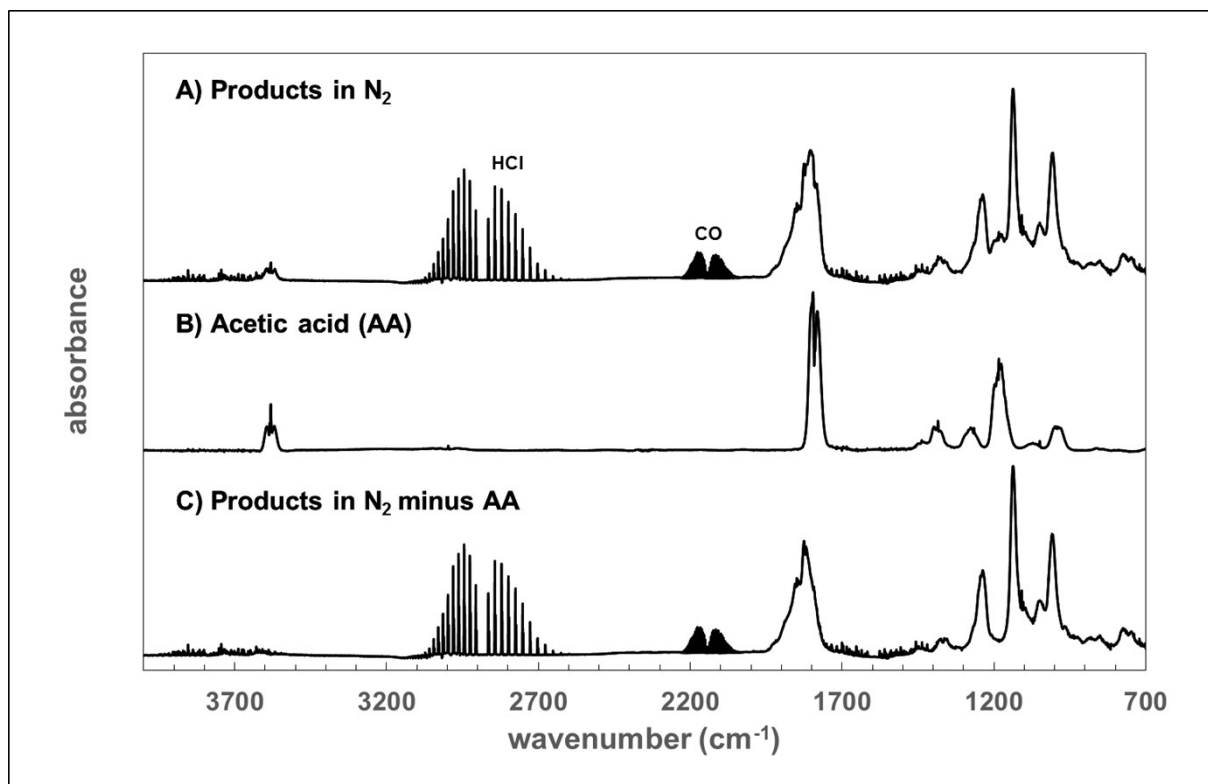


Fig. S2 Products formed in the irradiation of a propylene carbonate/ Cl_2 mixture in nitrogen. Trace (A) is the product spectrum after irradiation and subtraction of excess propylene carbonate, trace (B) is a reference spectrum of acetic acid and trace (C) is the residual product spectrum after subtraction of acetic acid from the spectrum in trace (A).

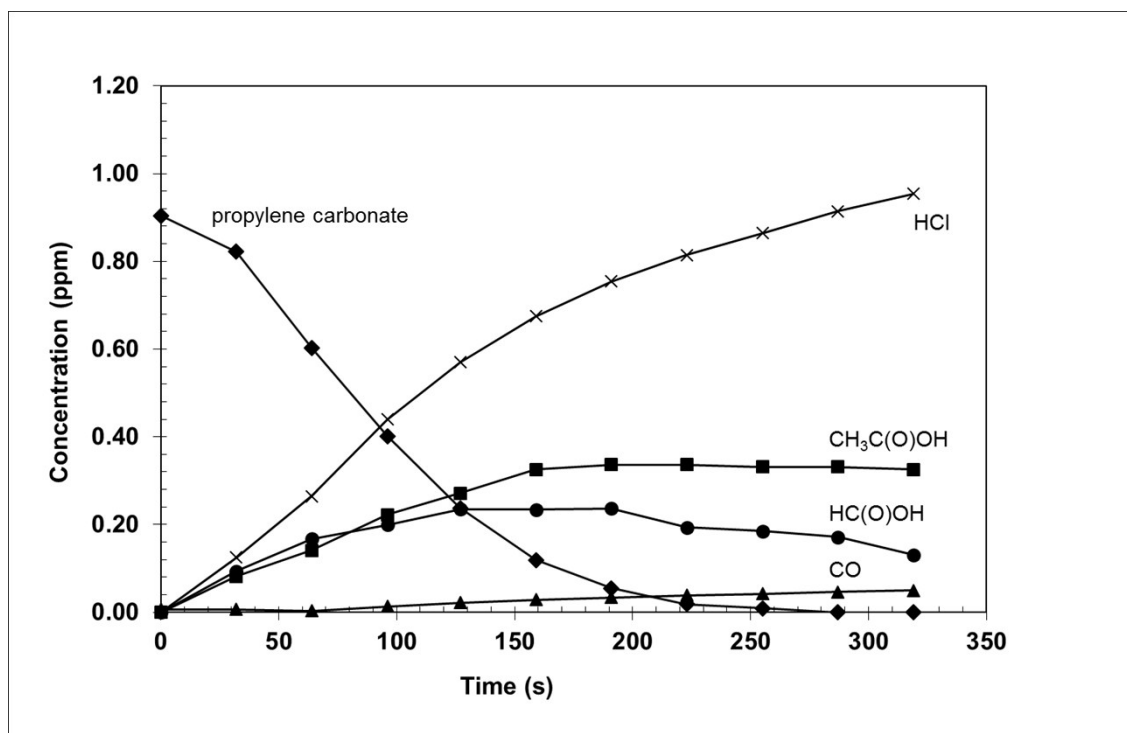


Fig. S3 Concentration-time profile for the decay of propylene carbonate and the formation of products on irradiation of a propylene carbonate/ Cl_2/N_2 mixture.

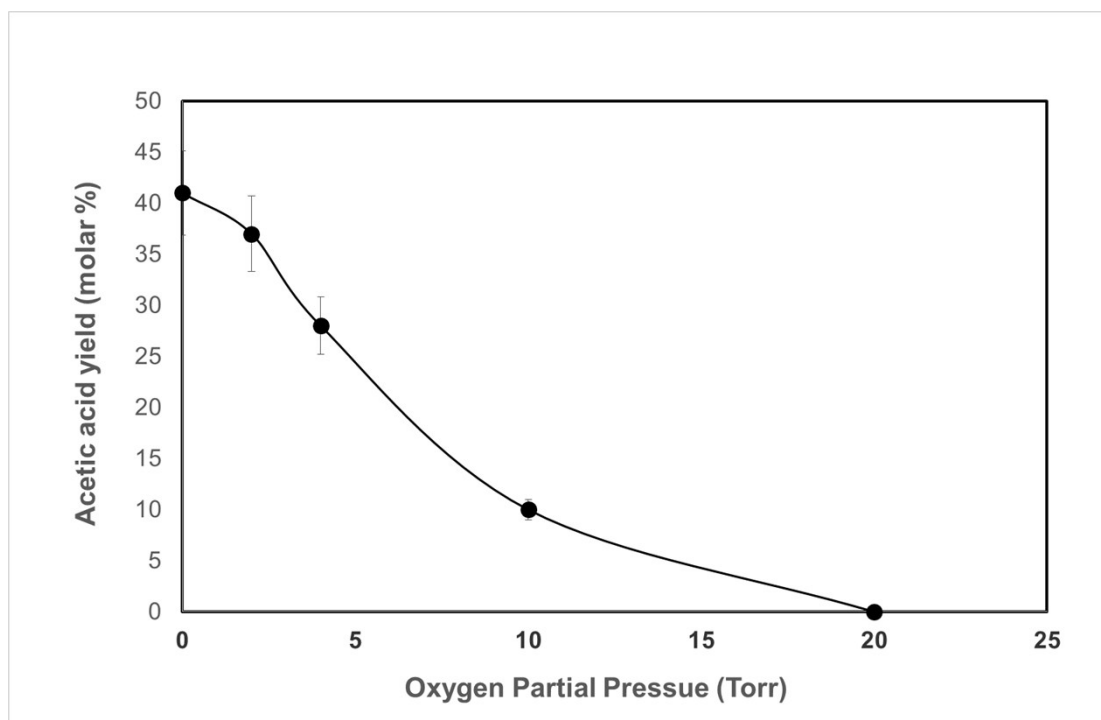
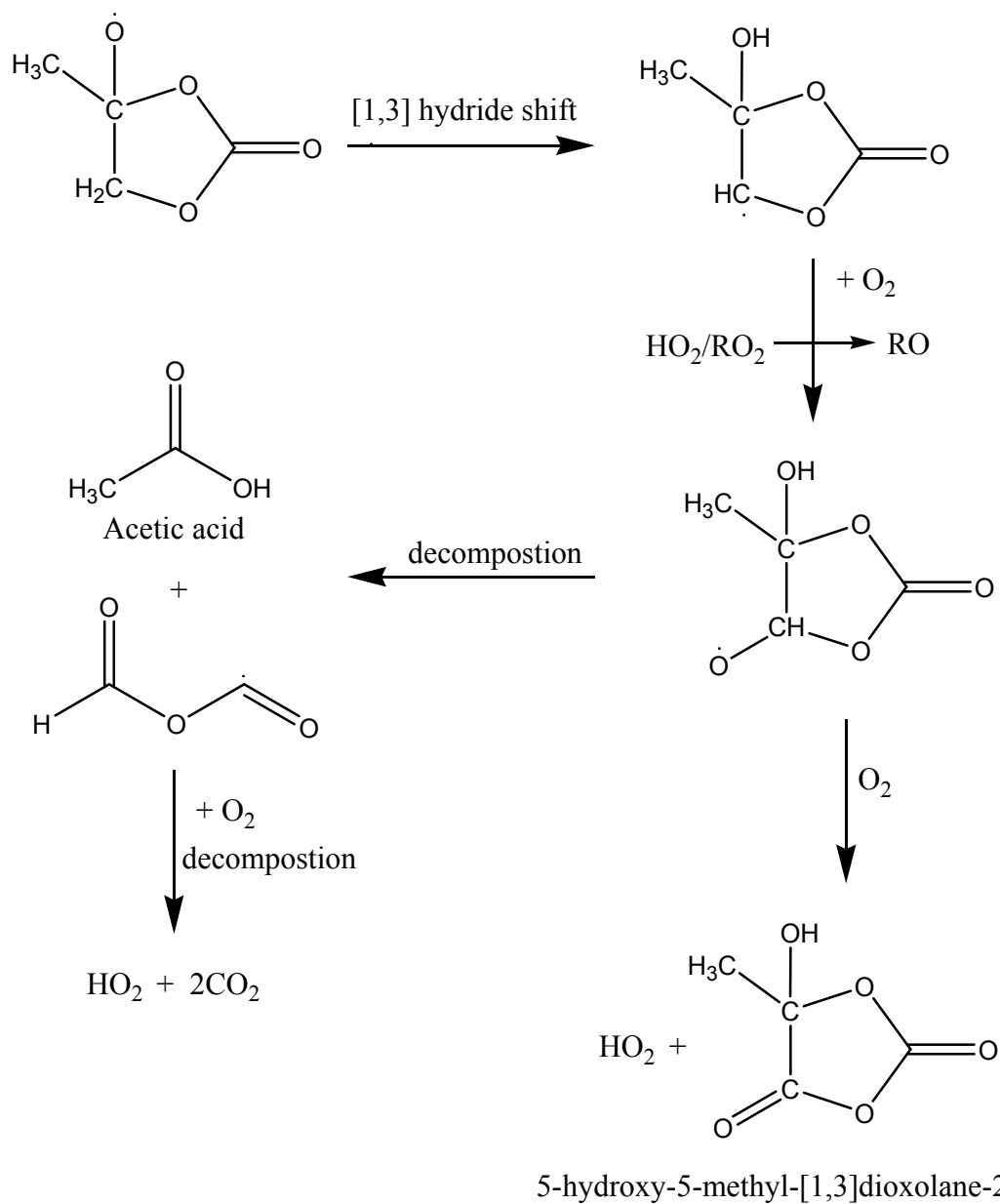


Fig. S4 Photolysis of a propylene carbonate/ Cl_2/N_2 mixture: Dependence of the acetic yields on the oxygen partial pressure.



Scheme S1 Possible mechanism, involving an α -ester rearrangement, for the formation of acetic acid in the Cl-atom initiated oxidation of propylene carbonate in N_2 .