

# **Thermo-Oxidative Conversion of PDC as a Molecular Model of Residual Feedstocks to Oxygen-Rich Chemicals**

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## **Supplementary information**

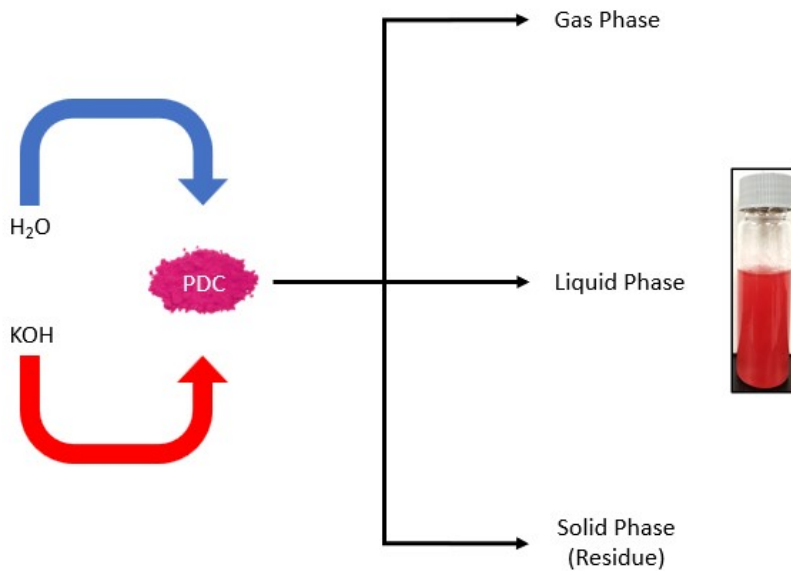


Fig. S1. Schematic showing the three major products of the reaction.

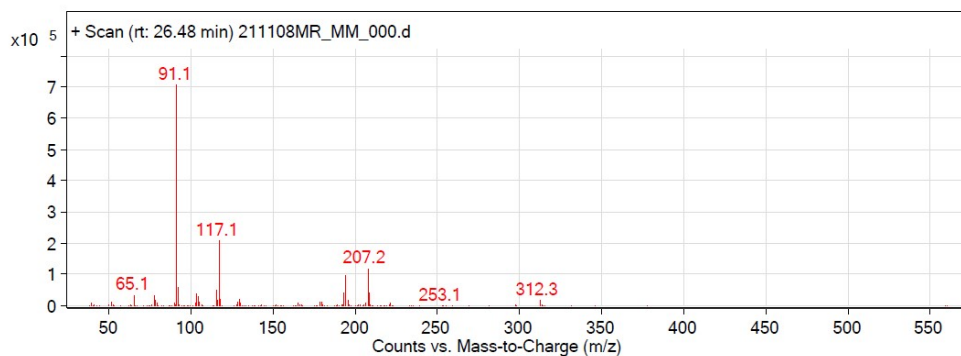


Fig. S2. Mass spectrum for the GCMS peak at retention time of 26.5 min in PDC.

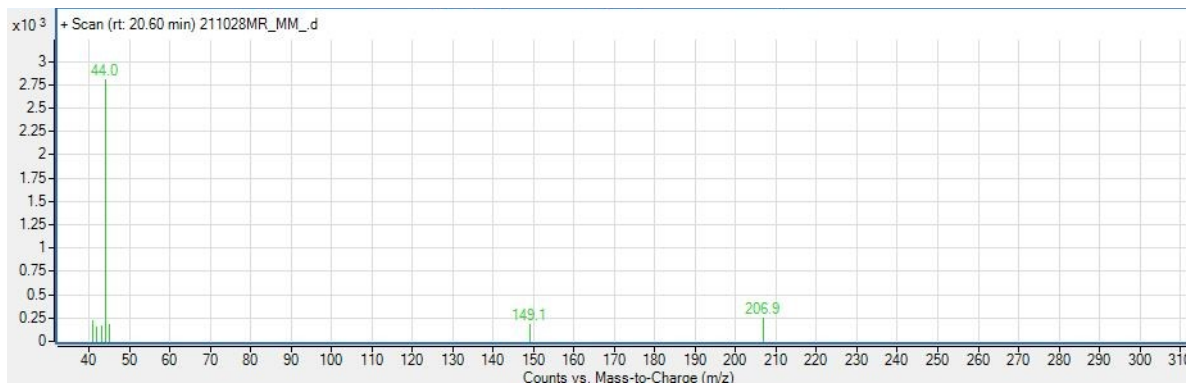


Fig. S3. Mass spectrum for the GCMS peak at retention time of 9 min in PDC.

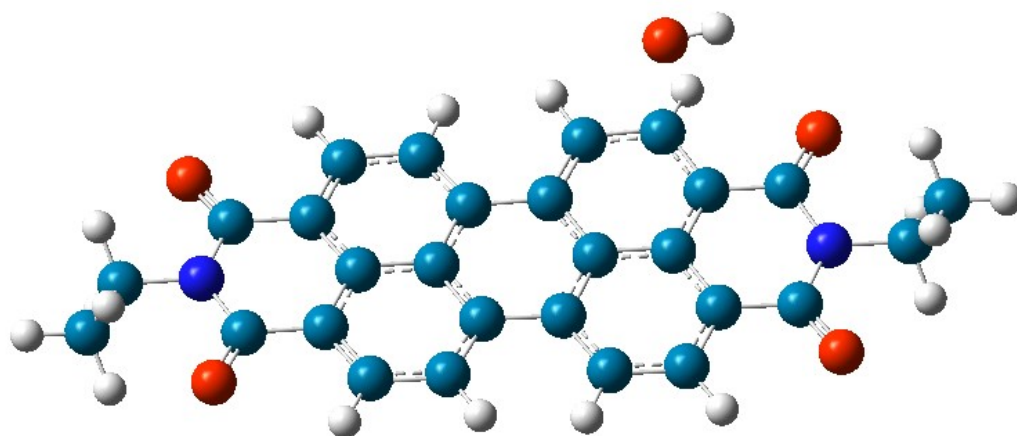


Fig. S4. Optimized geometry for TS1 at M062X/6-31+G(d,p) level of theory.

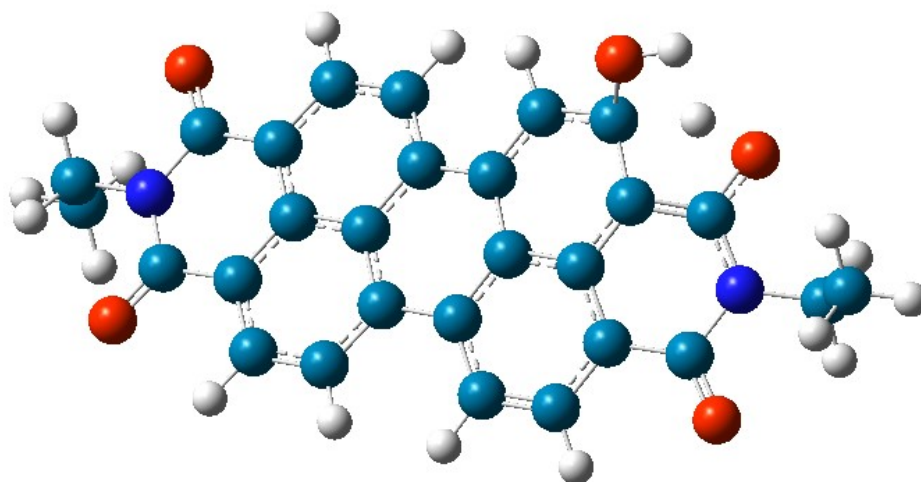


Fig. S5. Optimized geometry for TS2 at M062X/6-31+G(d,p) level of theory.

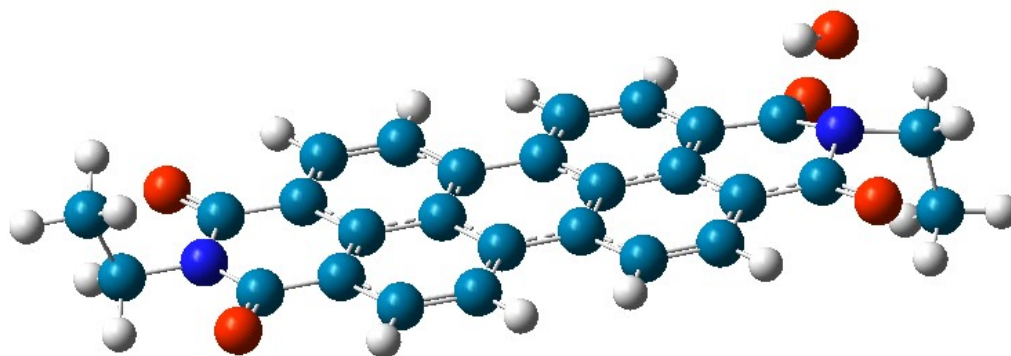


Fig. S6. Optimized geometry for TS3 at M062X/6-31+G(d,p) level of theory.

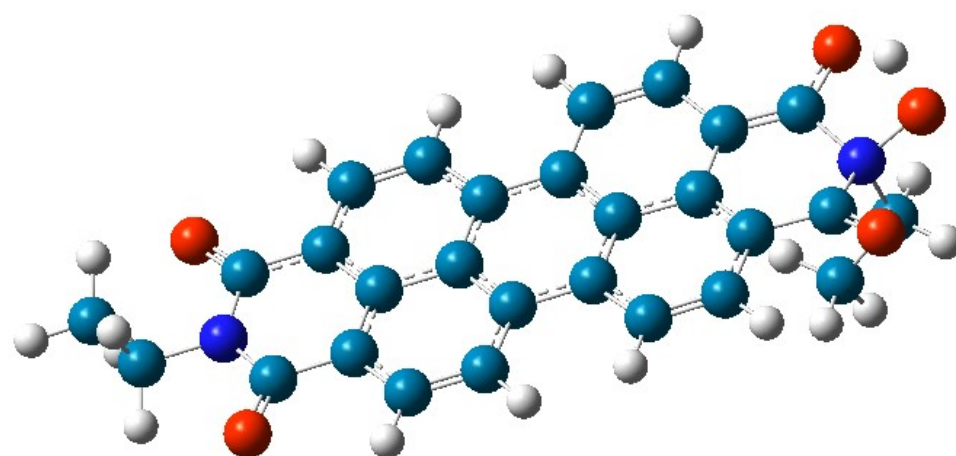


Fig. S7. Optimized geometry for TS4 at M062X/6-31+G(d,p) level of theory.

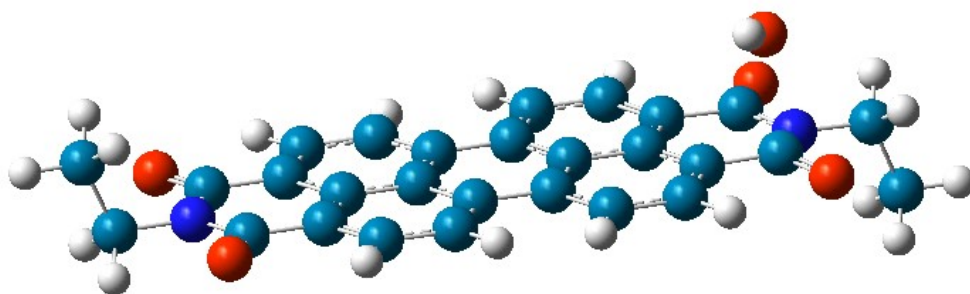


Fig. S8. Optimized geometry for TS5 at M062X/6-31+G(d,p) level of theory.

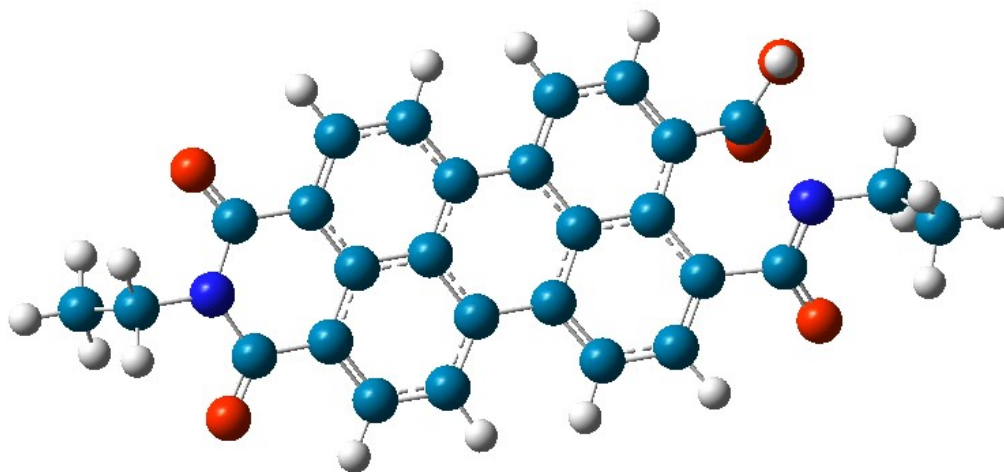


Fig. S9. Optimized geometry for TS6 at M062X/6-31+G(d,p) level of theory.

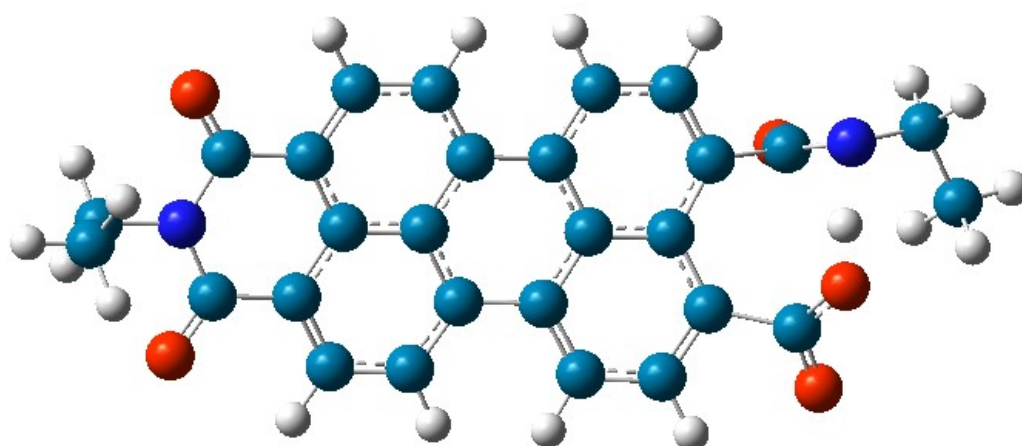


Fig. S10. Optimized geometry for TS7 at M062X/6-31+G(d,p) level of theory.

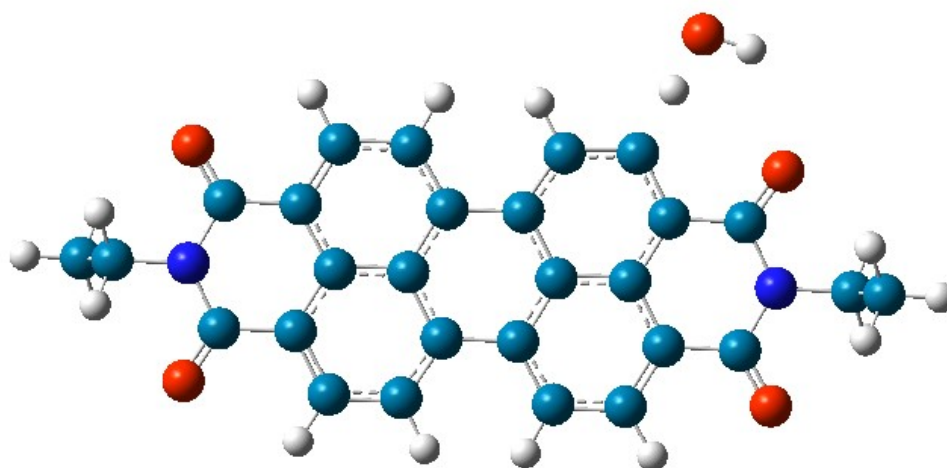


Fig. S11. Optimized geometry for TS8 at M062X/6-31+G(d,p) level of theory.