



## **Ozone oxidation of surface-adsorbed polycyclic aromatic hydrocarbons (PAHs): Role of PAH-surface interaction**

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We examine the effects of substrate on the oxidation of surface-bound anthracene and pyrene by gas-phase O<sub>3</sub> using density functional theory (B3LYP/6-31g\*\*). We find that the PAH-substrate interaction may result in the inhibition of some oxidation pathways involving nonplanar intermediates. The energy penalty for partial detachment from the surface is estimated and accounted for in the thermodynamic analysis of the reaction pathways. For anthracene, at least one oxidation pathway may be inhibited by strong interaction with the surface, thus impacting the rate of anthraquinone formation and possibly the observed rate of anthracene loss due to oxidation. Furthermore, the formation of other nonplanar products which have been proposed previously may be inhibited. When larger PAHs such as pyrene are surface-adsorbed, ring-opening reactions that proceed via the Criegee mechanism may be inhibited.