

Stereospecific Autocatalytic Surface Explosion Chemistry of Polycyclic Aromatic Hydrocarbons

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Additional data

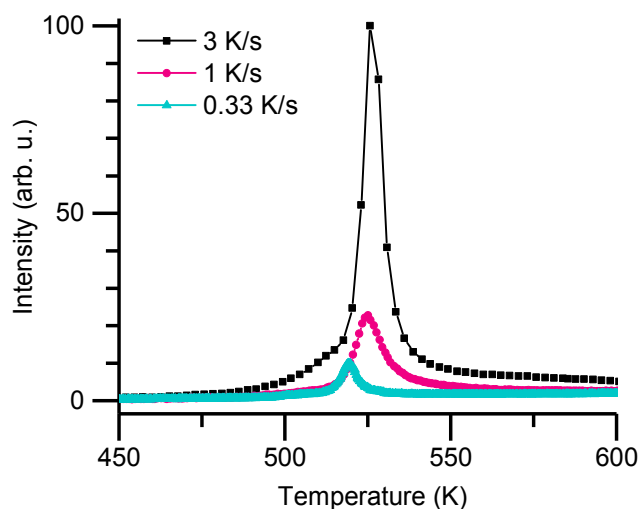


Figure S1: CO₂ (44 m/z) TPRS spectra 1 ML of Br[7]H on 1 ML of O/Cu(100) for different heating rates. The maximum of the TPR peak increases from 519 K for 0.33 K/s to 525 K for 1 K/s and 527 K for 3 K/s. At higher heat rates, the same amount of material desorbs in a shorter time, leading to a more intense signal.

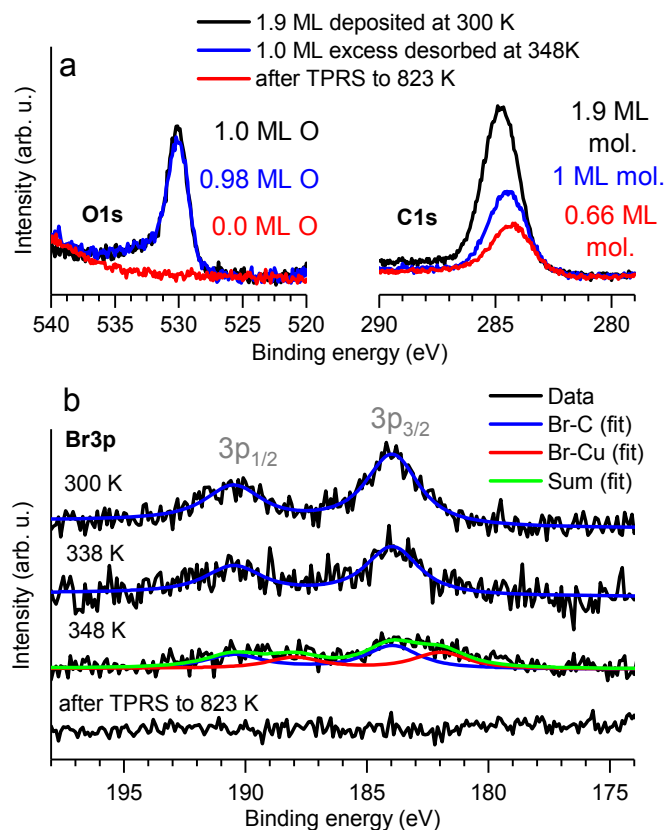


Figure S2: C1s, O1s and Br3p XP spectra of a nominal coverage of 1.9 ML diBr[7]H deposited on 1 ML O/Cu at 300 K. Annealing to 348 K leads to desorption of the molecules in the second layer. A saturated monolayer of molecules (defined as 1 ML) remains. After TPRS oxygen and bromine are completely desorbed. The equivalent of 0.66 ML of carbon remains.

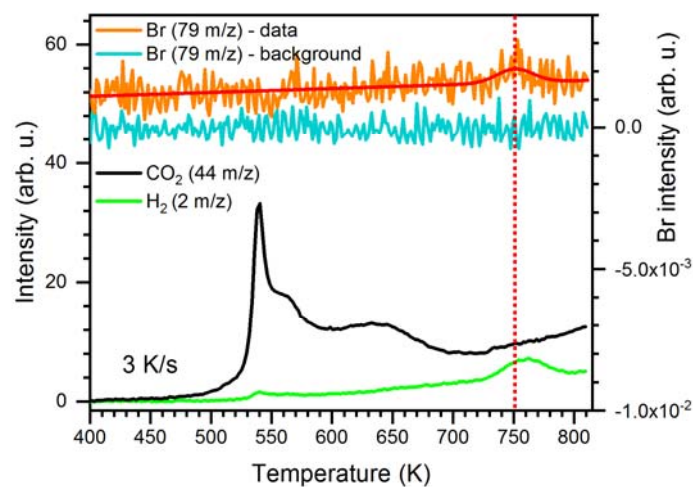


Figure S3: Br (79 m/z) TPR spectra for about 0.5 ML Br[7]H on 1 ML O/Cu. Br desorbs at 750 K. Molecular hydrogen (2 m/z) is detected at a slightly higher temperature. The heating rate is 3 K/s.

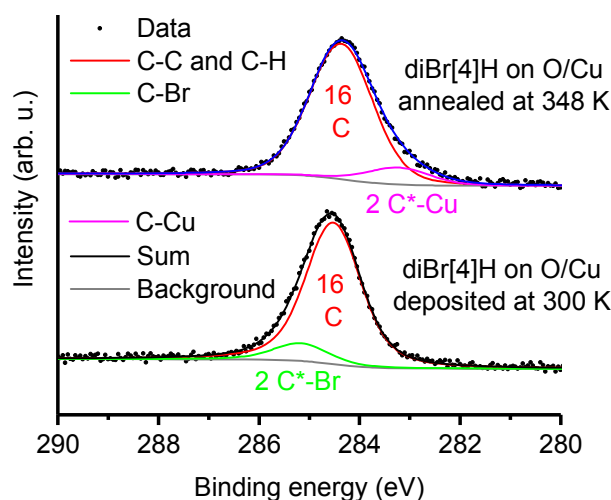


Figure S4: C1s XP spectra for 1 ML diBr[4]H deposited on O/Cu at 300 K and after annealing to 348 K. Before annealing the C1s spectrum exhibits a shoulder at 285.2 eV, indicative of C-Br. This shoulder is replaced by a shoulder at lower binding energy (283.3 eV) after annealing. Such low binding energy C1s species are characteristic for organometallic C-Cu bonds.³⁻⁵ The fits have been performed while keeping the relative intensities of the C-Br and C-Cu species fixed to 1/8, as expected for the stoichiometry of diBr[4]H.

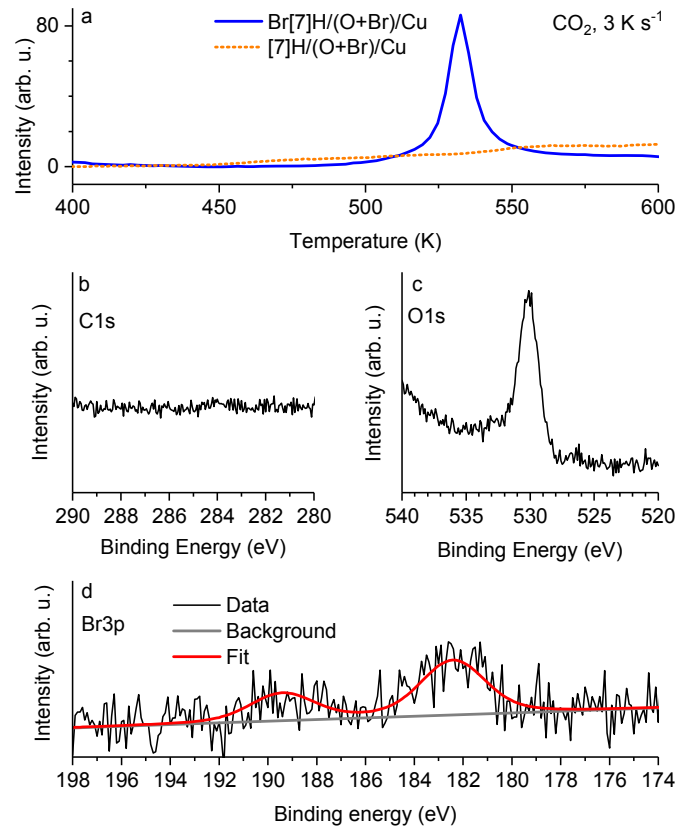


Figure S5: Control experiment showing that surface adsorbed Br is not responsible for the autocatalytic decomposition. (a) CO₂ TPR spectra of 1 ML [7]H and Br[7]H on 1 ML of Br doped O/Cu. Like on normal O/Cu, Br[7]H undergoes surface explosion and [7]H does not. (b-d) XPS spectra of a carbon free Br-doped O/Cu layer. It was prepared by annealing (633 K, 20 min) of 1 ML Br[7]H in 3×10^{-5} mbar O₂, followed by 5 min annealing (633 K). Under these conditions the carbon burns completely but the bromine remains.

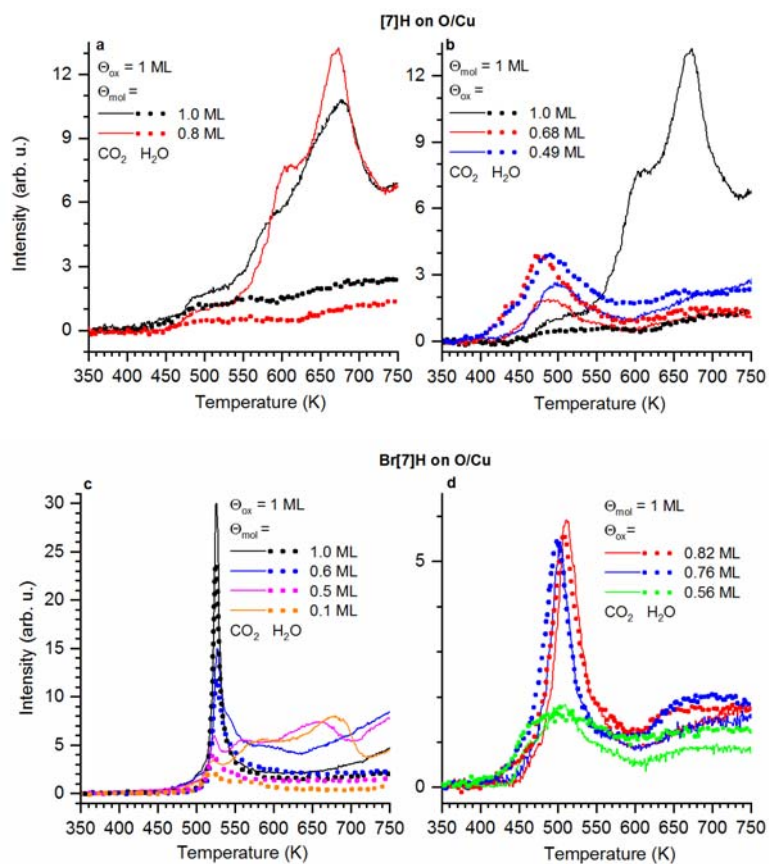


Figure S6: Comparison of simultaneously recorded CO_2 and H_2O TPR spectra for [7]H (a,b) and Br[7]H (c,d) as a function of molecular coverage (a,c) and oxygen coverage (b,d). The cases of 1 ML Br[7]H and of 1 ML [7]H on 1 ML O/Cu are compared in Figure 2.

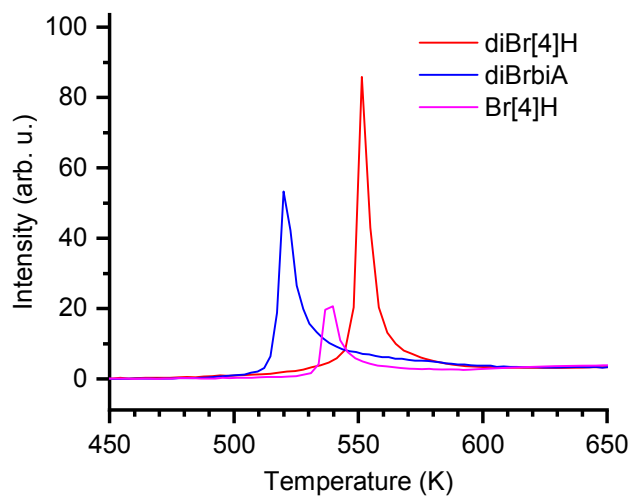


Figure S7: H₂O TPR spectra evidencing the autocatalytic decomposition of diBr[4]H, Br[4]H and diBrbiA. The heating rate is 3 K/s.

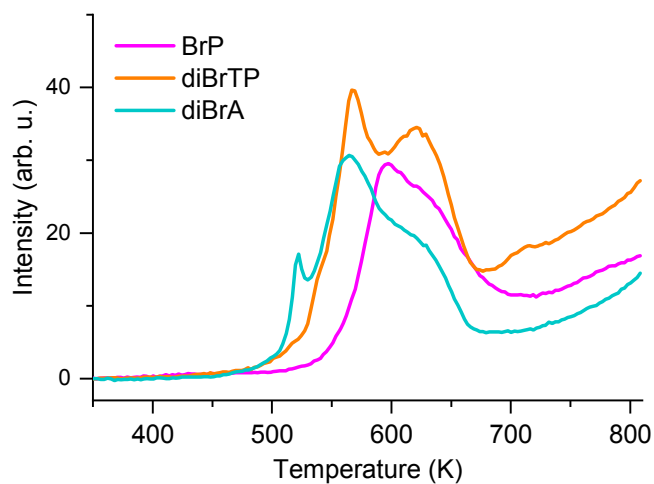


Figure S8: CO₂ TPR spectra evidencing the non-autocatalytic decomposition of BrP, diBrTP and diBrA. The heating rate is 3 K/s.

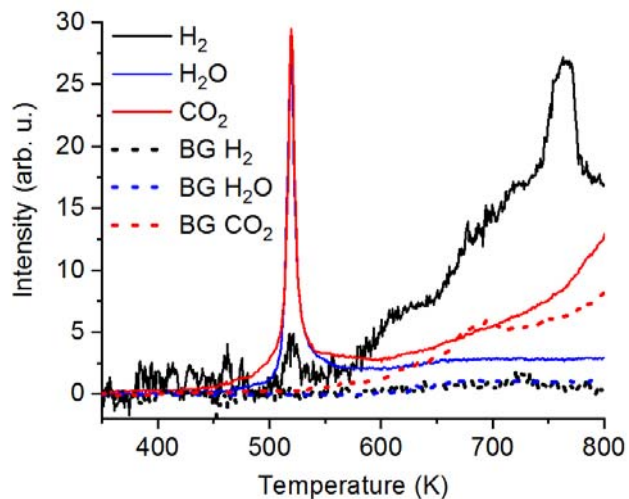


Figure S9: CO₂, H₂O and H₂ TPR spectra of 1 ML Br[7]H on 1 ML O. The heating rate is 1 K/s.

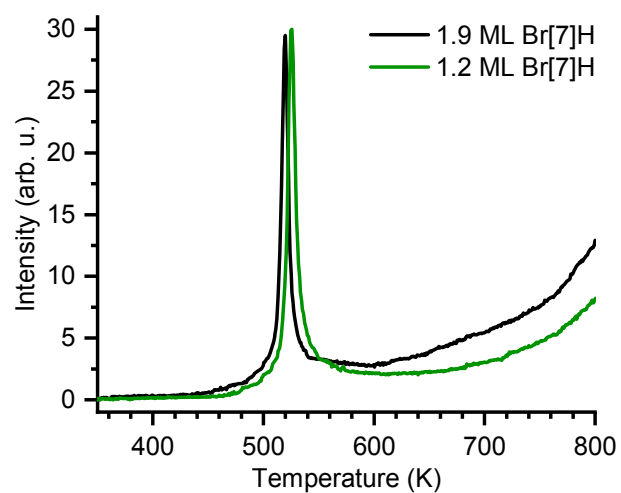


Figure S10: CO₂ (44 m/z) TPR spectra showing the autocatalytic decomposition of different nominal coverages (with respect to the coverage at 300 K) of Br[7]H on 1 ML of oxygen. The heating rate is 1 K/s.

References

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