

Oxygen as an Electron Scavenger: Its Role in Electron-Induced Activation of Coadsorbed Methane Embedded in Amorphous Solid Water

Sujith Ramakrishnan, Roey Sagi, Elishama Sorek, Rabin Rajan J. Methikkalam, and Micha Asscher*

Institute of Chemistry, Edmund J. Safra Campus, Givat-Ram

The Hebrew University, Jerusalem 91904, Israel

*Corresponding author e-mail: micha.asscher@mail.huji.ac.il

Supporting Information

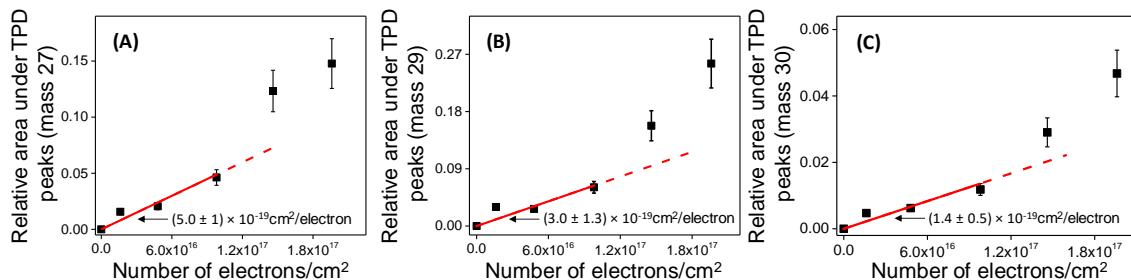


Figure S1 A-C. Integrated area under the TPD signals (corrected for the corresponding QMS sensitivity factors) at A) m/z = 27, B) m/z = 29, and C) m/z = 30 as a function of the number of 5 eV electrons (equivalent to the irradiation time) of pure methane (1ML=2.3L) sandwiched within two 50 ML D₂O layers along with the formation cross-sectional values obtained from the initial linear growth (in cm²/electron units). The Y-axis of all three figures was obtained by dividing the area under the TPD peak of each of the masses by the area obtained from one monolayer CH₄ sandwiched between two 50ML D₂O on Ru(0001) without irradiation. This way, together with correction for sensitivity factors, one obtains actual relative values of the products formation cross-section.

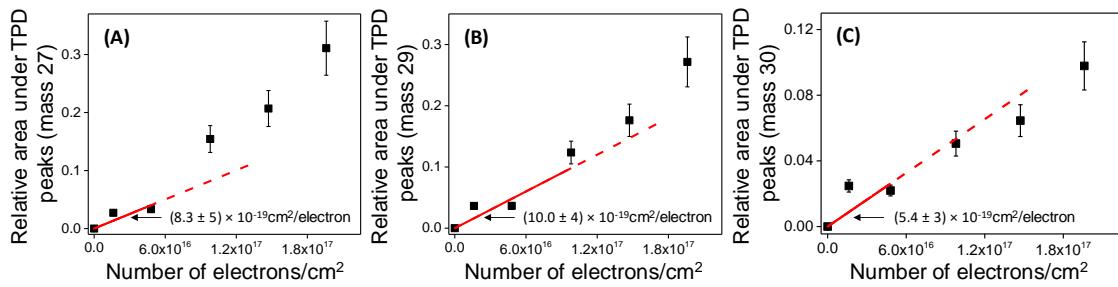


Figure S2 A-C. Integrated area under the TPD signals (corrected for the corresponding QMS sensitivity factors) at A) $m/z = 27$, B) $m/z = 29$, and C) $m/z = 30$ as a function of the number of 5 eV electrons (equivalent to the irradiation time) of a co-adsorbed system: 2.3L CH_4 + 2.5 L O_2 sandwiched within two 50 ML D_2O layers. The formation cross-sectional values were obtained from the initial linear growth.

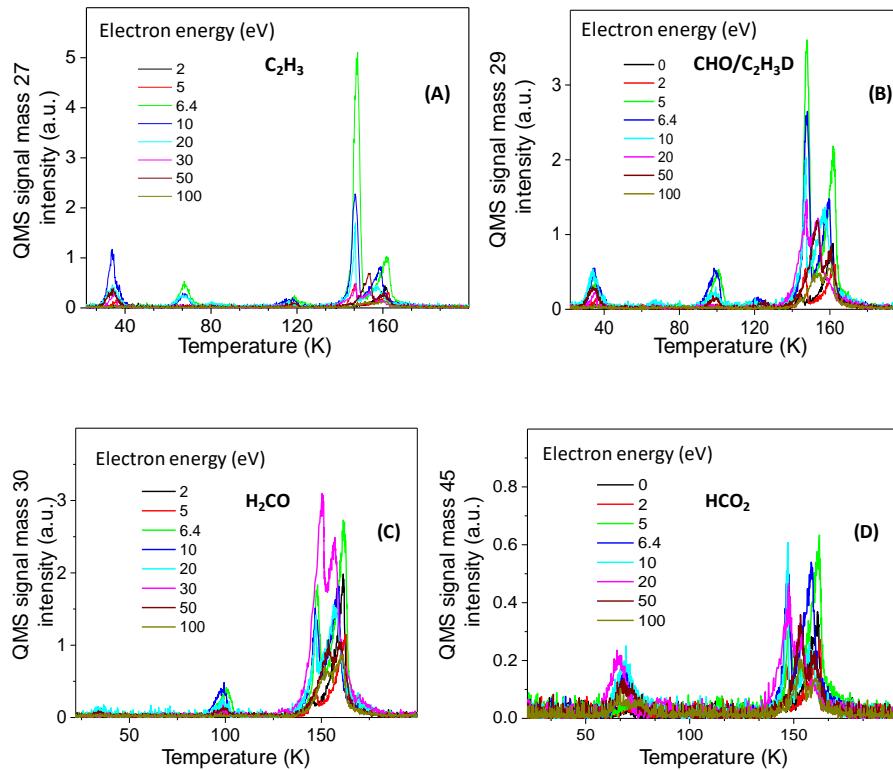


Figure S3 (A-D). TPD spectra of (A) $m/z = 27$, (B) $m/z = 29$, (C) $m/z = 30$ and (D) $m/z = 45$ obtained following irradiation by varying the electron energies of the 50 ML $\text{D}_2\text{O}|2.3 \text{ L } \text{CH}_4 + 2.5 \text{ L } \text{O}_2|50 \text{ ML } \text{D}_2\text{O}$ sample.

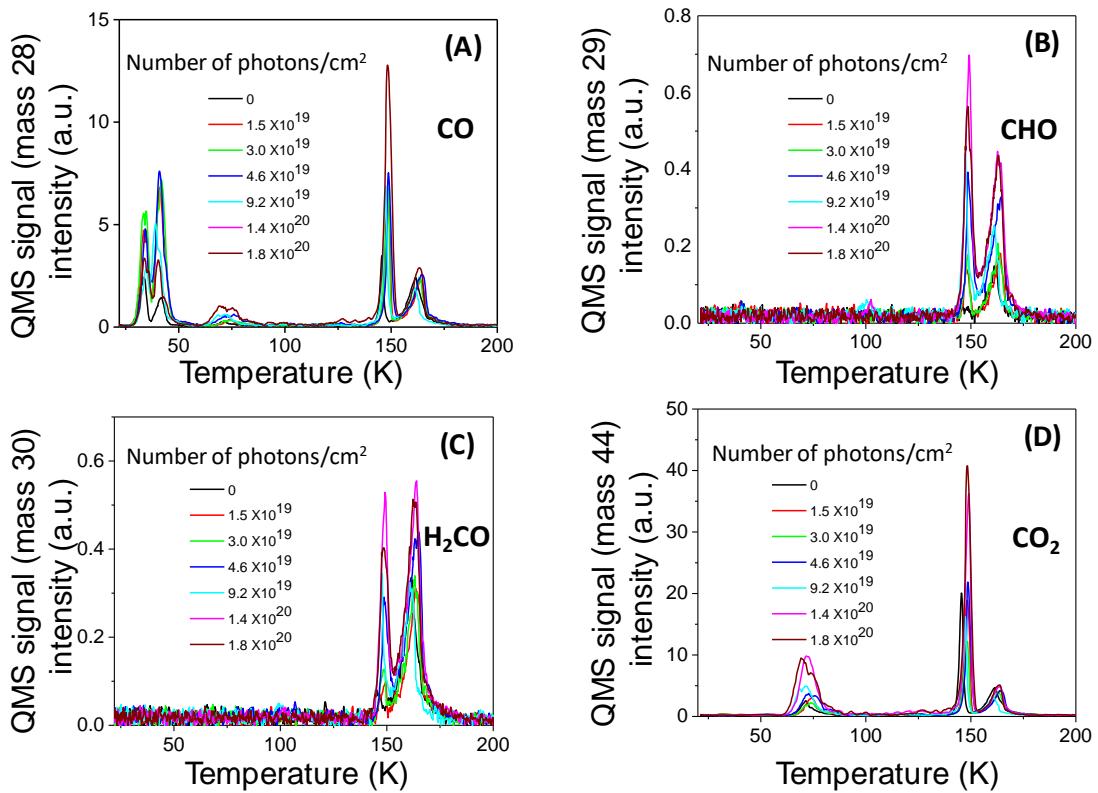


Figure S4 (A-D). TPD spectra (A)m/z = 28 (B)m/z = 29 (C)m/z = 30 and (D)m/z = 44 as a function of the number of photons. (Note: All the prepared samples were irradiated for 30 minutes with 5 eV electrons prior to their exposure to photons.)

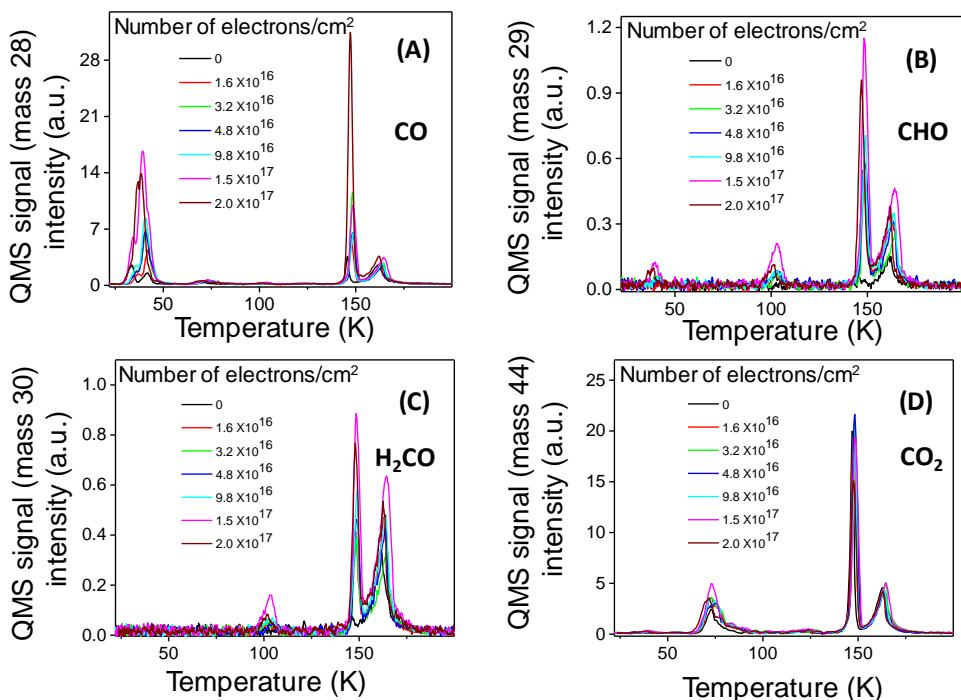


Figure S5 (A-D). TPD spectra (A) m/z = 28 (B) m/z = 29 (C) m/z =30 and (D) m/z = 44 as a function of the number of electrons. (Note: All the prepared samples were irradiated for 30 minutes with 248 nm photons prior to their exposure to electrons.)

Table ST1: A summary of the formation cross-sections (corrected for the corresponding QMS sensitivity factors) for the 5 eV electrons excitation of the ASW|2.3L CH₄|ASW and ASW|2.3L CH₄+10 L O₂ (co-adsorbed) |ASW system.

m/z (Product)	Cross-section (cm ² /electron)	
	ASW 2.3L CH ₄ ASW Ru(0001) ($\times 10^{-19}$)	ASW 2.3L CH ₄ +10 L O ₂ ASW Ru(0001) ($\times 10^{-19}$)
27	5.0±1.0	3.0±1.8
29	3.0±1.3	1.9±0.3
30	1.4±0.5	0.8±0.03
44	Not scanned	242±94
45	negligible	0.7±0.4
46	negligible	0.7±0.09