

Supplementary Material

Table S1 SMILES forms of the C_xH_yO_z species.

Molecular Formula	SMILES
CH ₃	[CH ₃]
CH ₂ O	C=O
CH ₃ O	C[O]
C ₂ H ₅ O	CO[CH ₂]
C ₂ H ₅ O ₂	COC[O]
C ₃ H ₇ O ₂	COCO[CH ₂]
C ₃ H ₇ O ₃	COCOC[O]
C ₄ H ₉ O ₃	COCOCO[CH ₂]
C ₄ H ₉ O ₄	COCOCOC[O]
C ₅ H ₁₁ O ₄	COCOCOCO[CH ₂]
C ₅ H ₁₁ O ₅	COCOCOCOC[O]
C ₆ H ₁₃ O ₅	COCOCOCOCO[CH ₂]
C ₆ H ₁₃ O ₆	COCOCOCOCOC[O]
PODE ₃	COCOCOCOC
PODE ₄	COCOCOCOCOC
PODE ₅	COCOCOCOCOCOC