Supporting Information

Product characterization and synergistic studies of in situ co-pyrolysis and catalytic pyrolysis of xylan and polyvinyl chloride

Tie Liu [a], Haodong Gao [a], Yu Liu [a], Zefeng Deng [b], Ying Zeng [a,*], Shiyuan Xu [a], Jing Hong [c], Jiahui Wang [a], Jiangle Zhang [a,*]

[a] College of Materials and Chemistry & Chemical Engineering, Chengdu University of Technology, Chengdu 610059, China.

[b] State Key Laboratory of Physical Chemistry of Solid Surfaces, Department of Chemistry, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, China.

[c] College of Chemistry and Materials Science, Sichuan Normal University, Chengdu 610066, China.

* Corresponding author.

E-mails addresses: zhangjiangle22@cdut.edu.cn (J.L. Zhang), zengy@cdut.edu.cn (Y. Zeng)

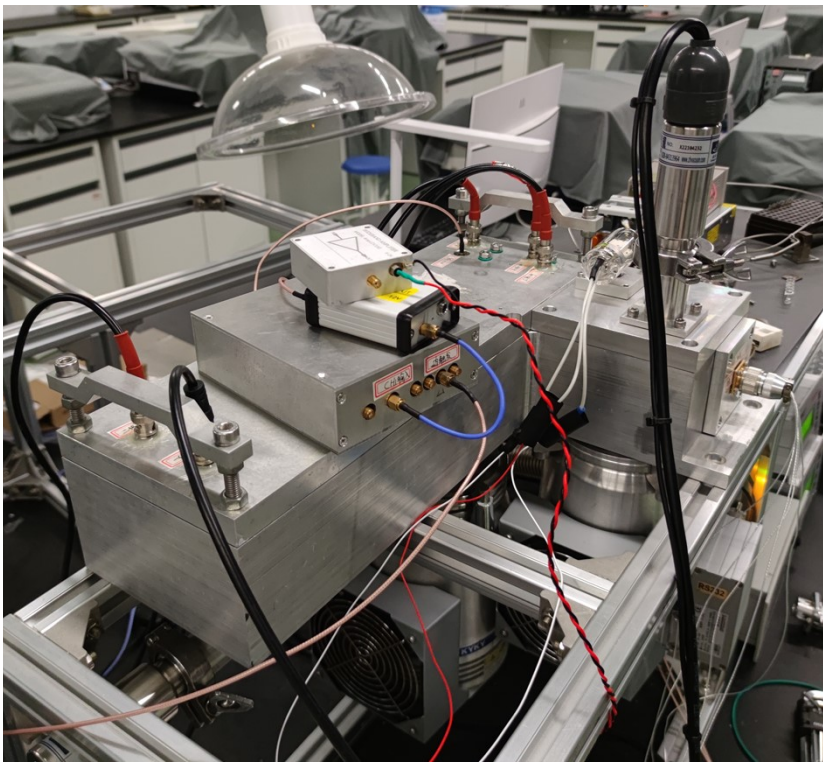


Fig. S1 Physical image of In-SituPy-TOFMS apparatus.

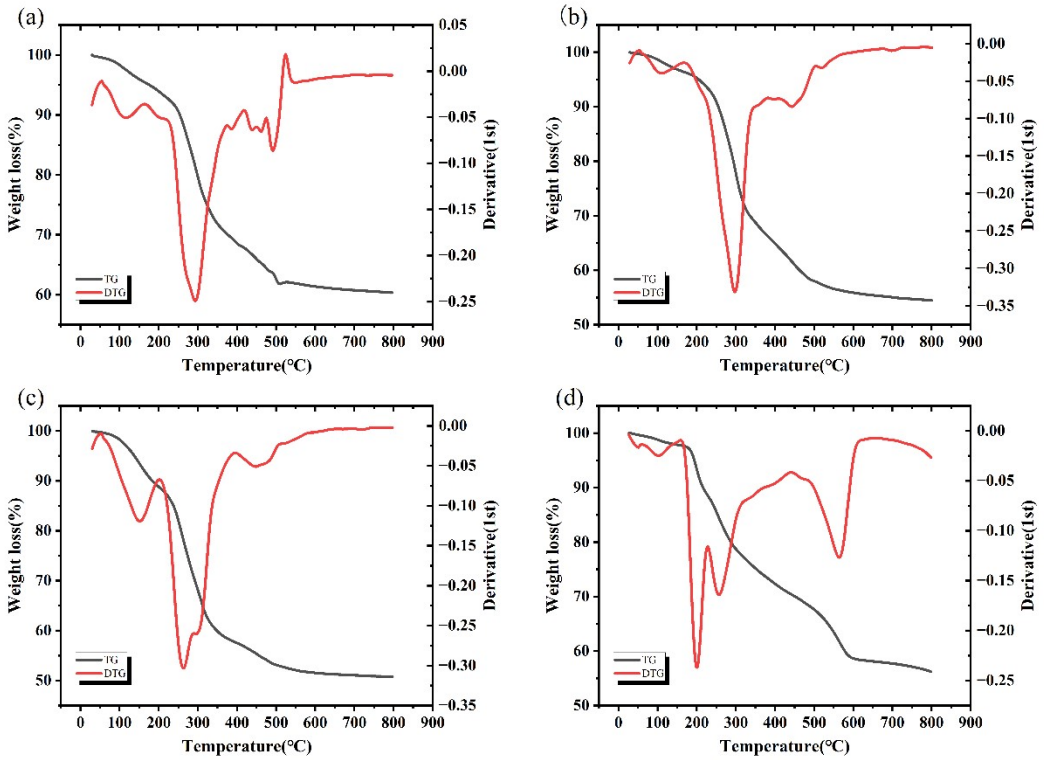


Fig. S2 The thermogravimetric (TG) / derivative thermogravimetry (DTG) curves of PVC and xylan under different catalyst conditions, (a)HZSM-5, (b)ZSM-5, (c)USY, (d)ZnO.

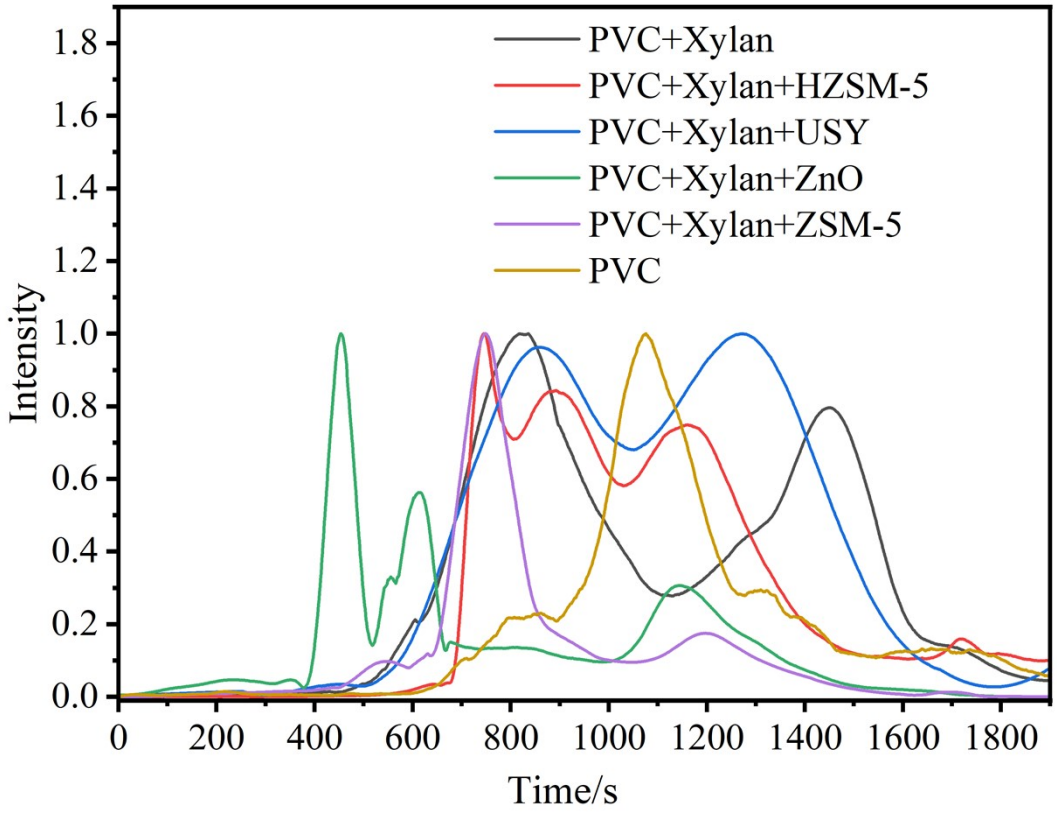
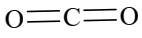
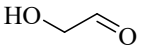
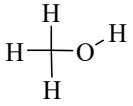
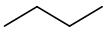
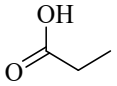
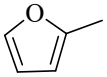
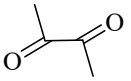
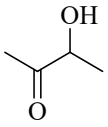
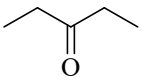
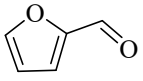
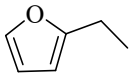
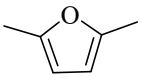
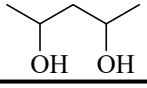


Fig. S3 TIC curves in the presence of different catalysts.

Table S1 Possible chemical attribution of the main products of xylan pyrolysis analyzed by In-SituPy-TOFMS.

m/z	Name	Formula	Category
44	carbon dioxide	CO_2	
44	acetic acid	C_2H_4O	
60	2-hydroxyacetaldehyde	$C_2H_4O_2$	
32	methanol	CH_4O	
42	prop-1-ene	C_3H_6	
44	acetaldehyde	C_2H_4O	
58	butane	C_4H_{10}	
68	furan	C_4H_4O	
74	propionic acid	$C_3H_6O_2$	
82	2-methylfuran	C_5H_6O	
86	biacetyl	$C_4H_6O_2$	
88	3-hydroxybutan-2-one	$C_4H_8O_2$	
96	pentan-3-one	$C_5H_{10}O$	
96	furan-2-carbaldehyde	$C_5H_4O_2$	
96	2-ethylfuran	C_6H_6O	
96	2,5-dimethylfuran	C_6H_6O	
104	pentane-2,4-diol	$C_5H_{12}O_2$	

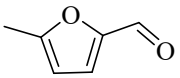
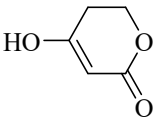
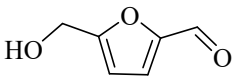
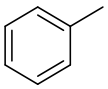
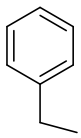
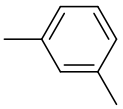
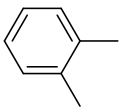
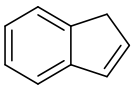
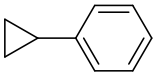
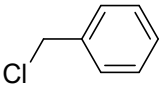
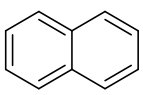
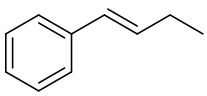
110	5-methylfuran-2-carbaldehyde	$C_6H_6O_2$	
114	4-Hydroxy-5,6-dihydro-2H-pyran-2-one	$C_4H_2O_4$	
126	5-(hydroxymethyl)furan-2-carbaldehyde	$C_6H_6O_3$	

Table S2 Possible chemical attribution of the main products of PVC pyrolysis analyzed by In-SituPy-TOFMS.

m/z	Name	Formula	Category
36	hydrogen chloride	HCl	
56	but-1-ene	C_4H_8	
66	cyclopenta-1,3-diene	C_5H_6	
78	benzene	C_6H_6	
92	toluene	C_7H_8	
94	cyclohepta-1,3-diene	C_7H_{10}	
106	ethylbenzene	C_8H_{10}	
106	m-xylene	C_8H_{10}	
106	o-xylene	C_8H_{10}	
116	1H-indene	C_9H_8	
118	cyclopropylbenzene	C_9H_{10}	
126	(chloromethyl)benzene	C_7H_7Cl	
128	naphthalene	$C_{10}H_8$	
132	(E)-but-1-en-1-ylbenzene	$C_{10}H_{12}$	

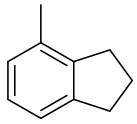
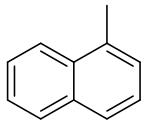
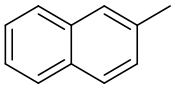
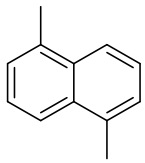
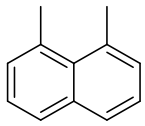
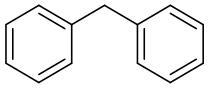
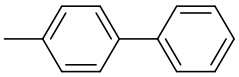
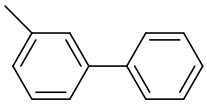
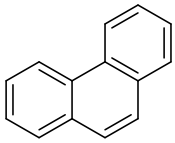
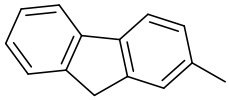
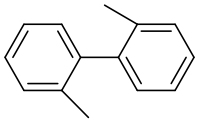
132	4-methyl-2,3-dihydro-1H-indene	$C_{10}H_{12}$	
142	1-methylnaphthalen	$C_{11}H_{10}$	
142	2-methylnaphthalene	$C_{11}H_{10}$	
156	1,5-dimethylnaphthalene	$C_{12}H_{12}$	
156	1,8-dimethylnaphthalene	$C_{12}H_{12}$	
168	diphenylmethane	$C_{13}H_{12}$	
168	4-methyl-1,1'-bipheny	$C_{13}H_{12}$	
168	3-methyl-1,1'-bipheny	$C_{13}H_{12}$	
178	phenanthrene	$C_{14}H_{10}$	
180	2-methyl-9H-fluorene	$C_{14}H_{12}$	
182	2,2'-dimethyl-1,1'-biphenyl	$C_{14}H_{14}$	

Table S3 Infrared band assignments for atomic cluster vibrational types.

Wave number (cm^{-1})	Functional group	Type
3670-3610,3400-3200	Alcohol, phenol O-H	stretching vibration
3560-3500，3000	carboxylic acid O-H	stretching vibration
3300-3270	≡C-H	stretching vibration
3090-3075	aromatic hydrocarbon C-H	stretching vibration
3100-2600	H-Cl	asymmetrical stretching vibration
3080-3020	=C-H	stretching vibration
2960-2850	-CH2-	stretching vibration
1680-1600	-C=C-/C=O	stretching vibration
1500-1400	aromatic hydrocarbon -C=C-	bending vibration
1470-1350	$-CH_3$	stretching vibration
1460	$-CH_2-$	scissoring vibration
1413	C-OH /O-C-O	stretching vibration
1033/917/842/786	C-O	stretching vibration
1000-960,940-900	=C-H	wagging vibration
1000-675	-C=C-	bending vibration
1000-650	AR-H=C-H	bending vibration
910-670	aromatic hydrocarbon C-H	twisting vibration
800-600	-C-Cl	stretching vibration

The 4000 - 3500 cm^{-1} region corresponds to O–H stretching vibrations, indicating the presence of alcohols, phenols, and carboxylic acids, while the 3054 - 2600 cm^{-1} range signifies C-H stretching vibrations in CH_4. The bands between 2404 - 2254 cm^{-1} (stretching) and at 670 cm^{-1} (bending) suggest the release of CO_2 via cleavage and secondary reactions involving -COOH and C=O groups. Absorptions within 2250 - 2000 cm^{-1} reflect C=O stretching in CO. The 1890 - 1612 cm^{-1} region corresponds to C=O double bonds in carboxylic acids, aldehydes, ketones, and their derivatives, whereas 1330 - 979 cm^{-1} indicates C-O stretching and O-H bending vibrations in esters and phenols.