Supporting Materials

Production of a renewable 1,3-diene containing a functional group from furfural-acetone adduct in a fixed-bed reactor

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Fig.S1 The N₂ adsorption isotherms and the pore size distribution plots of CeO₂ catalysts: (a) SiO₂,
(b)15Ce/SiO₂, (c) 20Ce/SiO₂, (d) 25Ce/SiO₂, (e) 30Ce/SiO₂, (f) 35Ce/SiO₂, (g) 40Ce/SiO₂.



Fig. S2 XPS patterns of ceria-based catalysts



Fig. S3 GC analysis of the products



Fig. S4 NH₃-TPD curves of the ceria-based catalysts. (b) is the magnification of dotted box in (a)

Catalyst	Temperature (°C)	Conversion (%)	Selectivity (%)	Yield (%)
PW/SiO ₂	300	100	79	79
Ag/SiO ₂	300	99	56	56
P/SiO ₂	300	100	6	6
Cu/SiO ₂	300	99	14	14
PMo/SiO ₂	300	100	38	38

Table S1 The dehydration over some acid catalysts

Catalyst weight: 0.40g; N_2 flow rate: 50 mL/min; the result data are averaged within 1 h.



Fig. S5 MASS of FAH (a) and target product (b)

(a): MS m/z: 138 (83), 123 (23), 95 (100), 91 (16), 81 (68), 77 (22), 67 (30), 55 (20), 43 (30);
Reference: J. Mol. Catal. B 2016, 126, 37–45; J. Chem. Soc., Perkin Trans. 1985, 1, 747–756
(b): MS m/z: 120 (42), 91 (100), 65 (18), 51 (8), 39 (14); Reference: Org. Biomol. Chem., 2010, 8, 2312–2315

The boiling point of FAH is evaluated as follows:

	Retention time (min) ^{<i>a</i>}	Boiling point/Pressure (°C/Torr) ^b			
F-diene	10.8	175/760			
FAH	13.4	-			
FA	13.7	135/30	116/10	110/9	104/5

Table S2 Retention time from GC data, and boiling point/pressure from SciFinder and Reaxys.

^{*a*}: GC with a ramp of 10 °C/min

^b: F-diene data comes from SciFinder and FA data from Reaxys.

(1) Based on retention time of GC data, the boiling point shows an order: FA≈FAH> F-diene.

(2) Based on lgP=A+B/T, A and B are constant, T is temperature (K),



Fig. S6 1/T as function of lgP

- (3) The boiling point of FA at atmosphere pressure (760 Torr) is 210 °C.
- (4) Therefore, the boiling point of FAH is around 200 °C (760 Torr).

Additionally, SciFinder suggests FA has a boiling point of approx. 175 °C (760 Torr). Considering Retention time of FA (10.8) and FAH (13.4), and GC with a ramp of 10 °C/min, the boiling point of FAH may be approx. 205 °C (760 Torr).