Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary information

Adsorption and Decarbonylation of Furfural over H-ZSM-5 zeolite: A DFT Study

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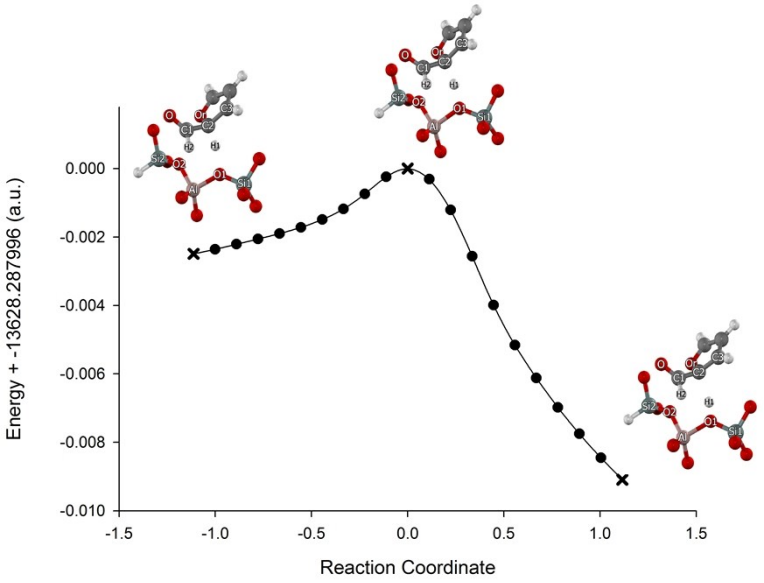
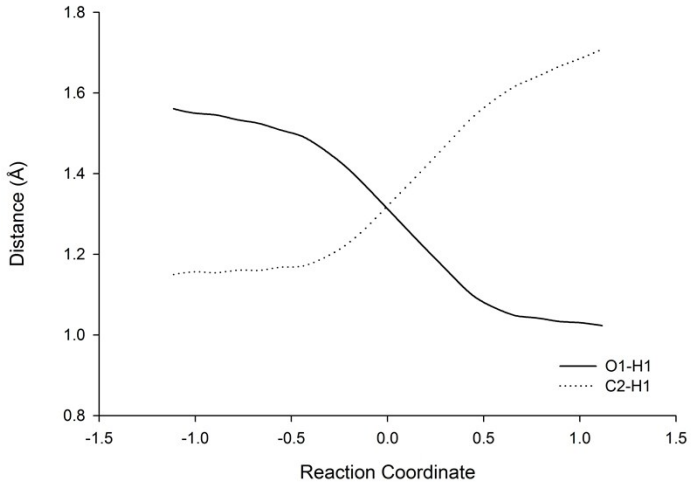
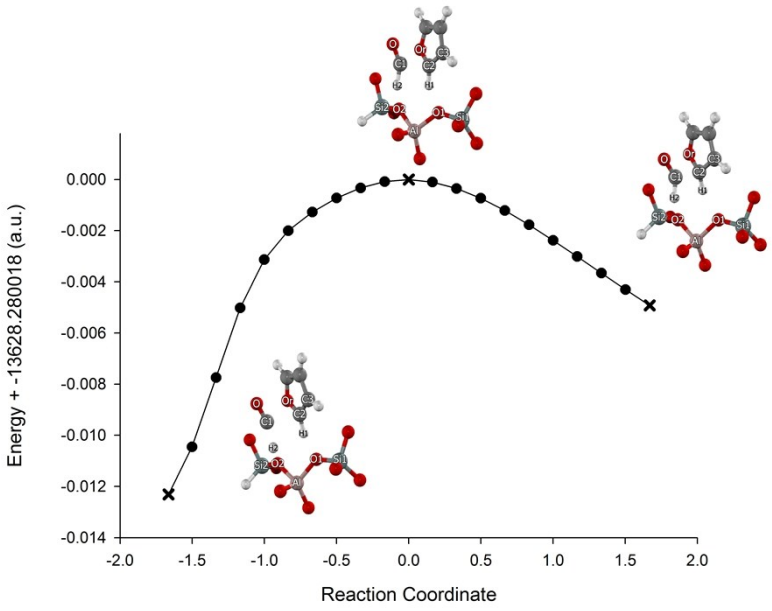


(a)

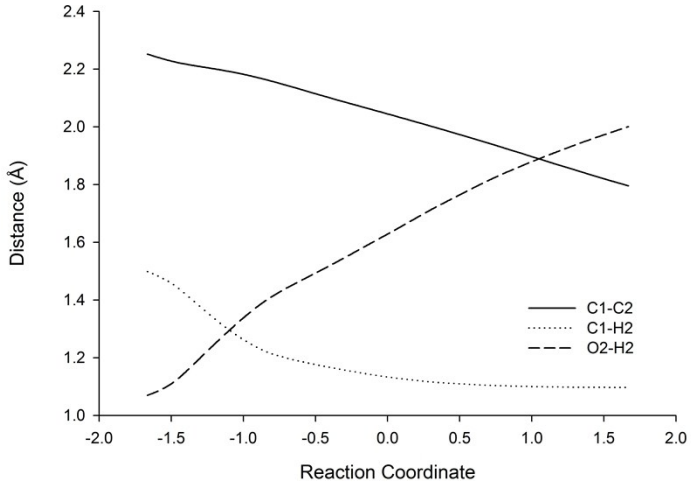


(c)

Fig. S1 Results from the IRC calculation for the protonation of furfural to produce the secondary carbocation intermediate over H-ZSM-5 zeolite. (a) Energy profile and structural changes; (b) Evolution of the O1-H1 and C1-H1 distances along the reaction coordinate.



(a)



(b)

Fig. S2 Results from the IRC calculation for the elimination of the CO group to the furan product over H-ZSM-5 zeolite. (a) Energy profile and structural changes; (b) Evolution of the C1-C2, C1-H2 and O2-H2 distances along the reaction coordinate.

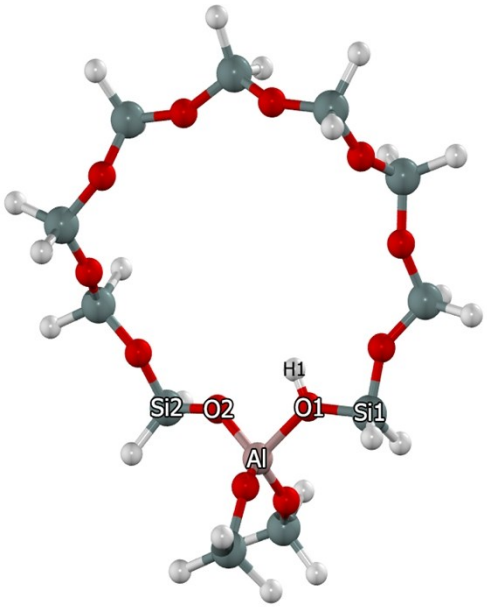


Fig. S3 The 12T cluster model of H-ZSM-5 zeolite.

Table S1. Relative energies from ΔE, ΔE_{zero}, ΔH and ΔG values at 298.15 K for the first pathway of the furfural decarbonylation on H-ZSM-5 as calculated on the M06-2X/6-31G(d,p) level of theory.

Reaction coordinates	Relative energies (kcal/mol)			
	ΔE	ΔE_{zero}	ΔH	ΔG
Ads_1	-19.6	-18.5	-18.1	-5.5
TS1_a	4.8(Ea1=24.4)	2.6(Ea1=21.1)	2.5(Ea1=20.6)	16.6 (Ea1=22.1)
Int1_a	-2.9	-2.1	-1.8	11.0
TS2_a	7.1(Ea2=10.0)	9.3(Ea2=11.4)	9.3 (Ea2=11.2)	23.3 (Ea2=12.3)
Prod	-15.7	-16.8	-15.4	-5.5

Table S2. Relative energies from ΔE, ΔE_{zero}, ΔH and ΔG values at 298.15 K for the second pathway of the furfural decarbonylation on H-ZSM-5 as calculated on the M06-2X/6-31G(d,p) level of theory.

Reaction coordinates	Relative energies (kcal/mol)			
	ΔE	ΔE_{zero}	ΔH	ΔG
Ads_1	-19.6	-18.5	-18.1	-5.5
TS1_b	9.3 (Ea1=28.9)	7.9 (Ea1=26.4)	7.8 (Ea1=25.9)	22.2 (Ea1=27.7)
Int1_b	7.1	7.3	7.7	20.8
TS2_b	25.6 (Ea2=18.5)	24.1 (Ea2=16.8)	24.4(Ea2=16.7)	37.2 (Ea2=16.4)
Int1_a	-2.9	-2.1	-1.8	11.0
TS2_a	7.1(Ea3=10.0)	9.3(Ea3=11.4)	9.3 (Ea3=11.2)	23.3 (Ea3=12.3)
Prod	-15.7	-16.8	-15.4	-5.5

Table S3. Relative energies from ΔE, ΔE_{zero}, ΔH and ΔG values at 298.15 K for the third pathway of the furfural decarbonylation on H-ZSM-5 as calculated on the M06-2X/6-31G(d,p) level of theory.

Reaction coordinates	Relative energies (kcal/mol)			
	ΔE	ΔE_{zero}	ΔH	ΔG
Ads_3	-30.7	-29.8	-29.8	-15.7
TS1_c	-15.5(Ea1=15.2)	-13.3(Ea1=16.5)	-13.8(Ea1=16.0)	1.1(Ea1=16.8)
Int1_c	-16.5	-13.4	-13.7	1.0
TS2_c	34.7 (Ea2=51.2)	32.7(Ea2=46.1)	32.6 (Ea2=46.3)	46.8 (Ea2=45.8)
Int1_b	7.1	7.3	7.7	20.8
TS2_b	25.6 (Ea3=18.5)	24.1 (Ea3=16.8)	24.4(Ea3=16.7)	37.2 (Ea3=16.4)
Int1_a	-2.9	-2.1	-1.8	11.0
TS2_a	7.1(Ea4=10.0)	9.3(Ea4=11.4)	9.3 (Ea4=11.2)	23.3 (Ea4=12.3)
Prod	-15.7	-16.8	-15.4	-5.5