Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

Theoretical Study on Reaction Mechanisms of Furfural Hydrogenation to Furfuryl Alcohol on Lewis Acidic BEA Zeolites: Effects of Defect Structure and Tetravalent Metals Substitution

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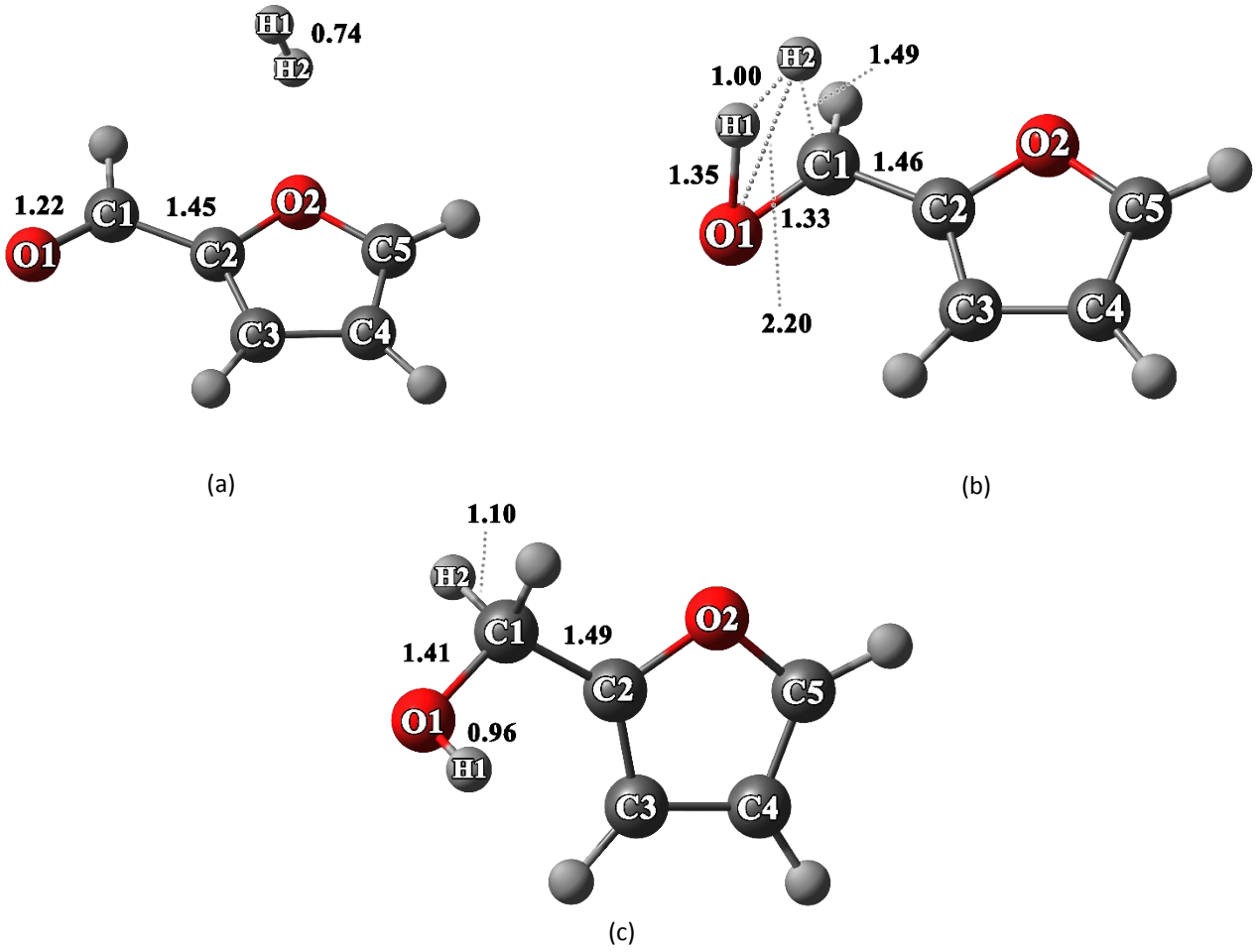

Figure S1. Optimized structures of (a) furfural and H_2 co-adsorption complex (Coads_uncatalyzed), (b) transition state (TS_uncatalyzed) and (c) furfural alcohol product (Prod_uncatalyzed) of the gas phase uncatalyzed reaction.

Table S1. Optimized geometrical parameters of the species involved in the furfural hydrogenation on perfect framework of Sn-BEA zeolite.

Parameter	Furfural adsorption (Ads)	Furfural and H_2 adsorption (Co-Ads)	Concerted TS (TS_C)	Furfuryl alcohol product (Prod)	Stepwise TS1 (TS1_S)	furylmethoxy intermediate (Int_S)	Stepwise TS2 (TS2_S)
				Distances (Å)			
Sn-OF	2.32	2.32	2.19	2.38	2.31	2.02	2.11
OF-C1	1.25	1.25	1.39	1.44	1.31	1.40	1.42
C1-C2	1.42	1.42	1.44	1.48	1.46	1.50	1.48
H1-H2	-	0.75	0.94	2.26	0.92	2.96	2.87
H1-C1	-	3.54	1.32	1.10	1.35	1.50	1.10
H2-OF	-	3.04	1.43	0.96	2.35	3.27	1.35
H2-O1	-	4.41	3.80	3.34	1.32	0.99	1.12
				Angles (°)			
O1-H2-OF	-	37.2	31.9	52.2	94.8	68.4	130.7
C1-OF-Sn	121.8	112.5	116.9	117.6	123.8	124.1	135.3
H1-C1-OF	-	70.0	104.7	110.6	110.9	113.9	109.8
C2-C1-H1	-	66.9	108.1	111.0	99.1	109.1	108.5

Table S2. Optimized geometrical parameters of the species involved in the furfural hydrogenation on defect framework of Sn-BEA zeolite.

Parameter	Furfural adsorption (Ads)	Furfural and H_2 adsorption (Co-Ads)	Furfuryl alcohol product (Prod)	Stepwise TS1 (TS1_S)	furylmethoxy intermediate (Int_S)	Stepwise TS2 (TS2_S)
			Distances (Å)			
Sn-OF	2.32	2.32	2.25	2.15	2.00	2.17
OF-C1	1.25	1.25	1.45	1.31	1.41	1.42
C1-C2	1.42	1.42	1.48	1.44	1.48	1.49
H1-H2	-	0.75	2.87	0.88	3.14	3.25
H1-C1	-	3.69	1.10	1.47	1.10	1.10
H2-OF	-	2.80	0.98	2.36	2.76	1.24
H2-O1	-	4.47	2.69	1.46	0.97	1.23
			Angles (°)			
O1-H2-OF	-	36.1	82.7	90.8	87.1	134.1
C1-OF-Sn	118.1	118.1	120.9	123.2	120.0	139.4
H1-C1-OF	-	68.6	103.7	106.9	108.2	108.3
C2-C1-H1	-	69.9	112.7	103.8	109.9	110.0