Electronic Supplementary Material (ESI) for RSC Advances.

Table S1

Optimized geometrical parameters (bond lengths in pm and angles in degrees) of hydrogen bonding of cluster models calculated at the B3LYP/6-311++G** and *w*P97XD/6-311++G**level of theory.

B3LYP/6-311++G**							
8T-ZSM-5 …Benzene		8T-Al-ZSM-5 …Benzene		8T-ZSM-5 …Phenol		8T-Al-ZSM-5 …Phenol	
C_B-H_B…O_{Z1}	282.1 (150.1*)	C_B-H_B…O_{Z2}	264.2 (123.8)	O_P-H_P…O_{Z1}	221.2 (177.7)	O_{Z1}-H_Z…O_P	158.2 (163.9)
		C_B-H_B…O_{Z2}	288.4 (114.5)			O_P-H_P…O_{Z2}	173.7 (145.6)
		O_{Z1}-H_Z…л	264.6 (165.0)				
*w*P97XD/6-311++G**							
8T-ZSM-5 …Benzene		8T-Al-ZSM-5 …Benzene		8T-ZSM-5 …Phenol		8T-Al-ZSM-5 …Phenol	
C_B-H_B…O_{Z1}	253.0 (122.0)	C_B-H_B…O_{Z2}	264.9 (113.8)	O_P-H_P…O_{Z1}	203.6 (169.5)	O_{Z1}-H_Z…O_P	163.6 (159.5)
		C_B-H_B…O_{Z2}	272.6 (111.2)			O_P-H_P…O_{Z2}	181.1 (142.8)
		O_{Z1}-H_Z…л	235.8 (141.3)				

*The angle of hydrogen bondings are available in parentheses.

Table S2

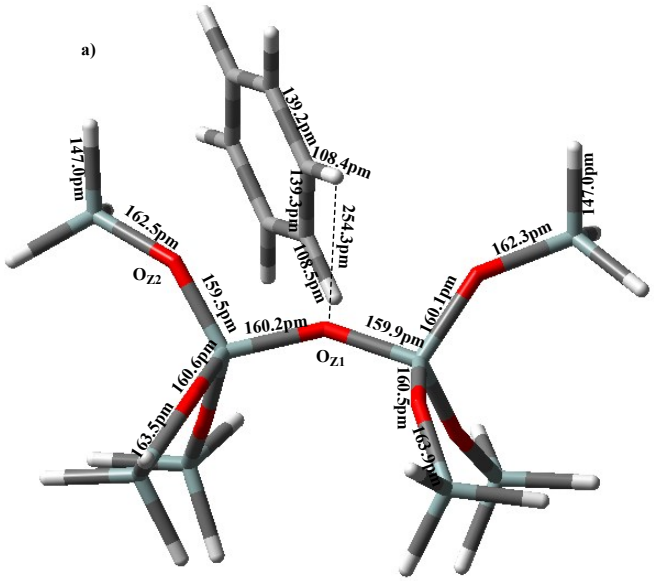
Selected calculated ^{17}O, ^{1}H, and ^{27}Al NMR chemical shifts (in ppm), quadrupole coupling constant (in MHz for ^{17}O and ^{27}Al nuclei, and KHz for ^{2}H nuclei), and asymmetry parameter for ^{17}O, ^{2}H, and ^{27}Al nuclei before and after adsorption in the cluster models at the B3LYP/DZVP2 level of theory. The values in parentheses represent the calculated data before the adsorption.

cluster models	nucleus	δ_{iso}(Cal.)	C_Q	η_Q
8T-ZSM-5…Benzene	H_B	8.10(7.58)	208.22(213.11)	0.07(0.07)
	O_{Z1}	63.76(60.18)	6.55(6.680)	0.27(0.23)
	O_{Z2}	11.11(8.88)	6.58(6.63)	0.31(0.30)
	Si	-74.78(-73.53)		
8T-Al-ZSM-5…Benzene	H_B	8.11(7.58)	207.15(213.11)	0.05(0.07)
	O_{Z1}	59.47(56.38)	8.73(8.92)	0.84(0.80)
	H_Z	4.16(3.96)	291.96(305.10)	0.10(0.09)
	O_{Z2}	-1.89(-4.38)	4.15(4.15)	0.72(0.80)
	Al	76.20(80.71)	19.15(19.93)	0.20(0.17)
	Si	-76.72(-76.17)		
8T-ZSM-5…Phenol	O_P	100.42(96.54)	11.08(11.21)	0.83(0.94)
	H_P	5.90(3.75)	300.91(322.70)	0.14(0.13)
	O_{Z1}	72.55(60.18)	6.08(6.68)	0.44(0.23)
	O_{Z2}	12.49(8.88)	6.57(6.63)	0.29(0.30)
	Si	-75.18(-73.53)		
8T-Al-ZSM-5…Phenol	O_P	99.89(96.54)	10.11(11.21)	0.89(0.94)
	H_P	8.99 (3.75)	240.73(322.70)	0.11(0.13)
	O_{Z1}	59.60(56.38)	6.78(8.92)	0.96(0.80)
	H_Z	11.04(3.96)	174.20(305.10)	0.20(0.09)
	O_{Z2}	15.04(-4.38)	4.05(4.15)	0.85(0.80)
	Al	78.39(80.71)	15.82(19.93)	0.08(0.17)
	Si	-74.71(-76.17)		

Table S3

Selected calculated ^{17}O, ^{1}H, and ^{27}Al NMR chemical shifts (in ppm), quadrupole coupling constant (in MHz for ^{17}O and ^{27}Al nuclei, and KHz for ^{2}H nuclei), and asymmetry parameter for ^{17}O, ^{2}H, and ^{27}Al nuclei before and after adsorption in the cluster models at the *w*B97XD/DZVP2 level of theory. The values in parentheses represent the calculated data before the adsorption.

cluster models	nucleus	δ_{iso}(Cal.)	C_Q	η_Q
8T-ZSM-5…Benzene	H_B	8.20(7.61)	212.48(216.21)	0.06(0.07)
	O_{Z1}	61.64(53.06)	6.79(6.89)	0.21(0.21)
	O_{Z2}	7.96(1.38)	6.78(6.90)	0.30(0.25)
	Si	-72.98(-72.12)		
8T-Al-ZSM-5…Benzene	H_B	8.10(7.61)	211.73(216.21)	0.05(0.07)
	O_{Z1}	58.41(46.63)	8.62(8.90)	0.90(0.81)
	H_Z	3.48(3.75)	299.79(320.22)	0.11(0.09)
	O_{Z2}	-6.63(-13.22)	4.32(4.34)	0.60(0.69)
	Al	74.67(76.04)	18.16(19.75)	0.27(0.19)
	Si	-76.72(-74.77)		
8T-ZSM-5…Phenol	O_P	86.60(80.08)	11.02(11.37)	0.82(0.91)
	H_P	6.18(3.63)	309.74(341.01)	0.13(0.13)
	O_{Z1}	71.93(53.06)	6.27(6.89)	0.41(0.21)
	O_{Z2}	5.98 (1.38)	6.81(6.90)	0.24(0.25)
	Si	-74.90(-72.12)		
8T-Al-ZSM-5…Phenol	O_P	84.69(80.08)	10.32(11.37)	0.88(0.91)
	H_P	7.90(3.63)	267.97(341.01)	0.10(0.13)
	O_{Z1}	48.81(46.63)	6.84(8.90)	1.02(0.81)
	H_Z	10.10(3.75)	204.39(320.22)	0.15(0.09)
	O_{Z2}	6.46(-13.22)	4.25 (4.34)	0.71(0.69)
	Al	73.03(76.04)	16.02(19.75)	0.11(0.19)
	Si	-75.97(-74.77)		


a)
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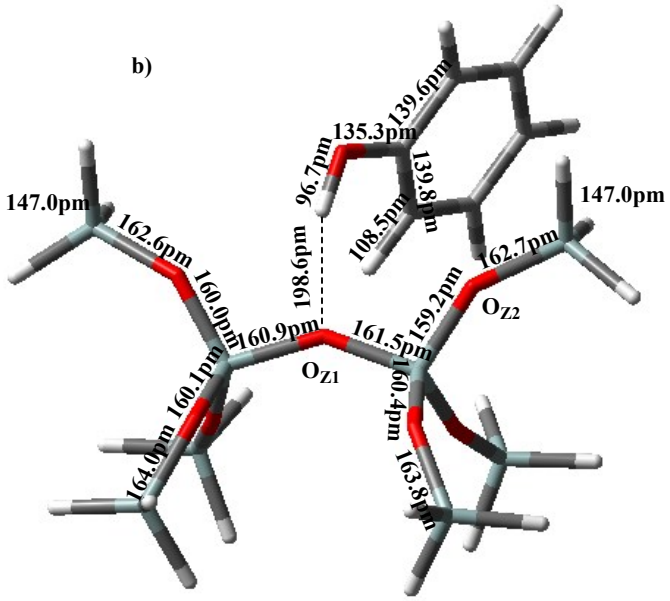
147.0pm
139.3pm
254.3pm
162.5pm
108.5pm
147.0pm
162.3pm
O_{Z2}
159.5pm
160.2pm
159.9pm
160.1pm
O_{Z1}
160.6pm
160.5pm
163.5pm


b)
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135.3pm
96.7pm
139.8pm
147.0pm
147.0pm
108.5pm
162.6pm
198.6pm
162.7pm
160.0pm
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O_{Z2}
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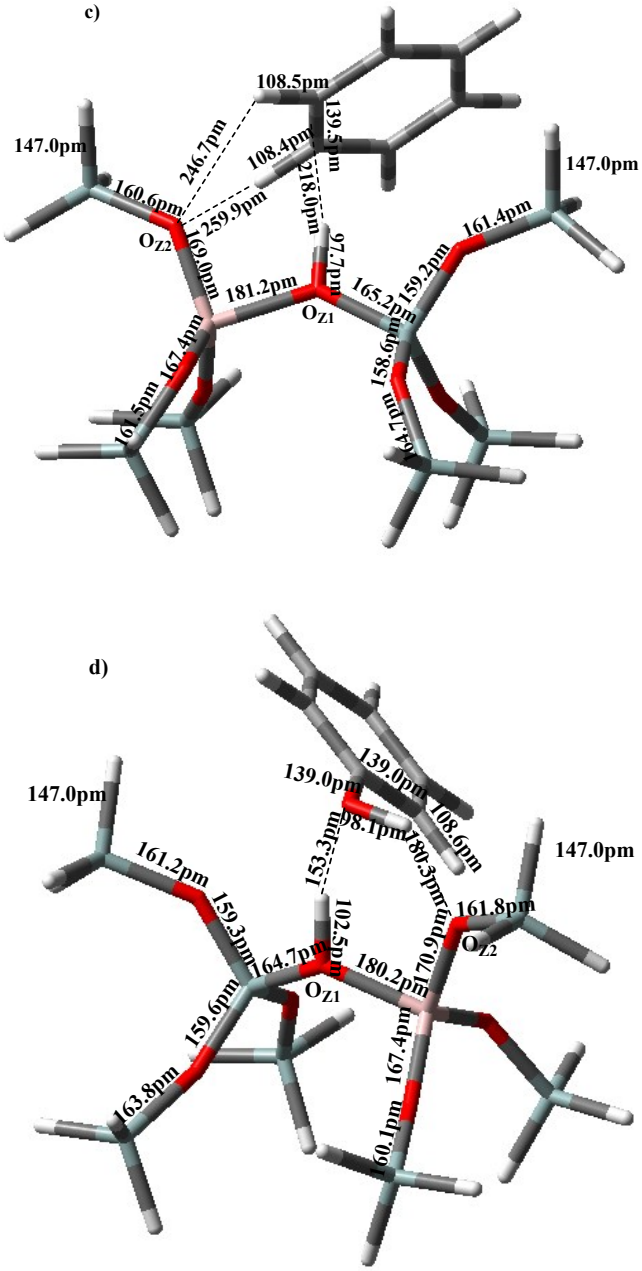

Fig. S1. Representation of optimized geometries structures in: a)8T-ZSM-5…Benzene, b)8T-ZSM-5…Phenol, c)8T-Al-ZSM-5…Benzene, and d)8T-Al-ZSM-5…Phenol cluster models at M06-2X/6-311++G** level.