Supplementary Information

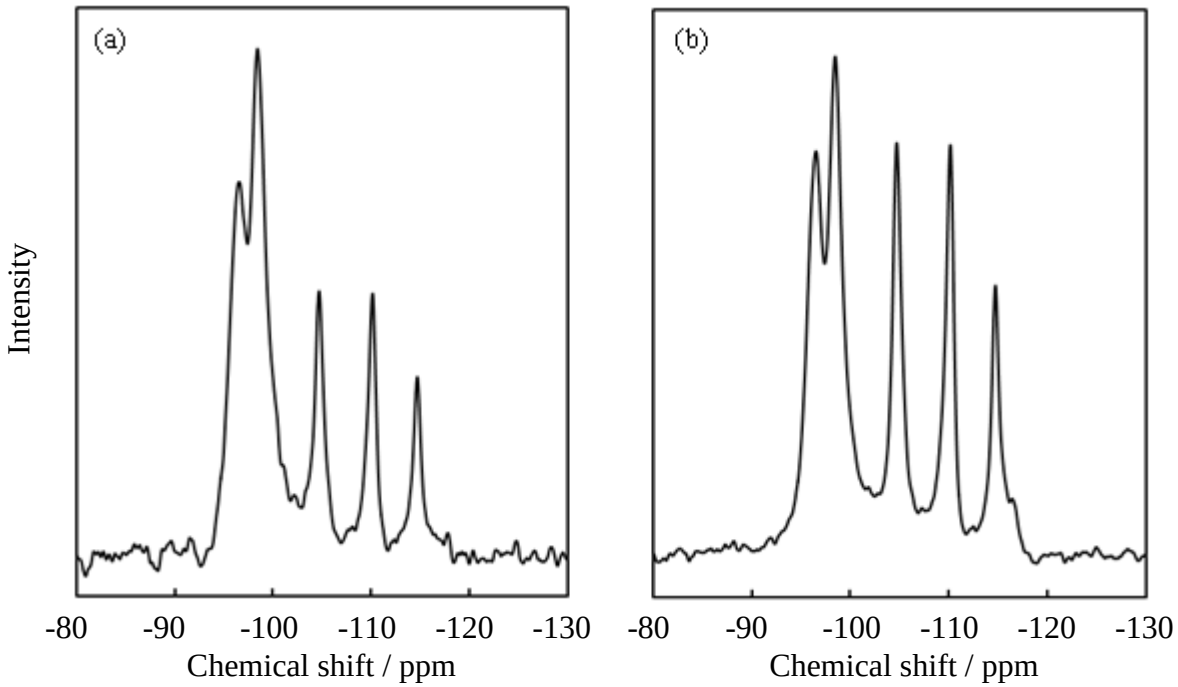

Figure S1 ^{29}Si CP-MAS NMR spectra of as-synthesized HUS-7 (Sample 7) measured at different contact times: (a) 0.5 μs and (b) 4.0 μs.

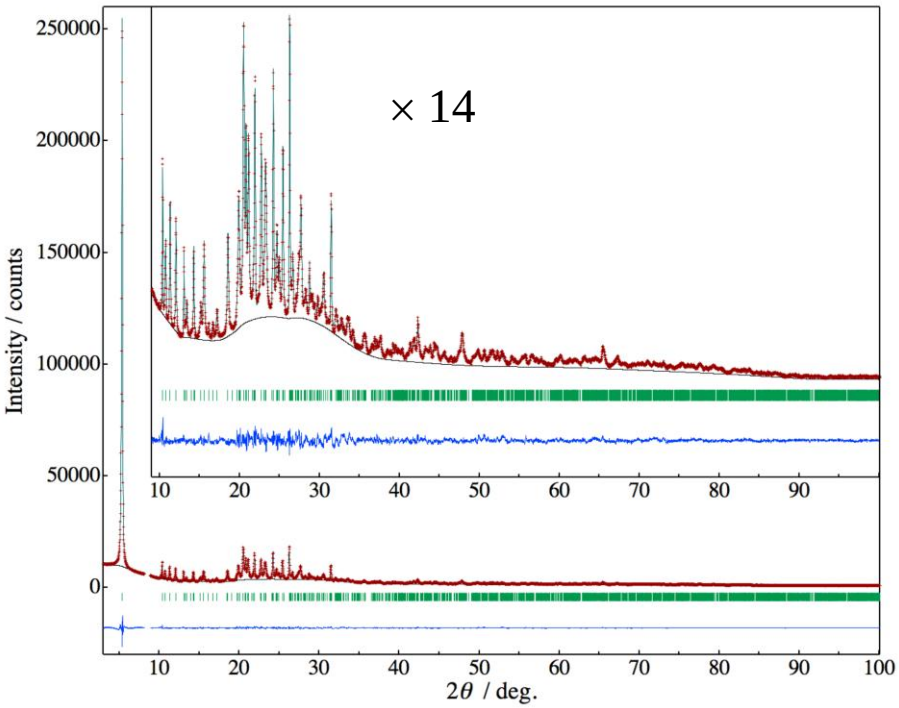

Figure S2 Observed pattern (red crosses), calculated pattern (light blue solid line), and difference pattern (blue) obtained by Rietveld refinement for HUS-7. The tick marks (green) denote the peak positions of possible Bragg reflections. The inset shows magnified patterns from 10° to 100°.

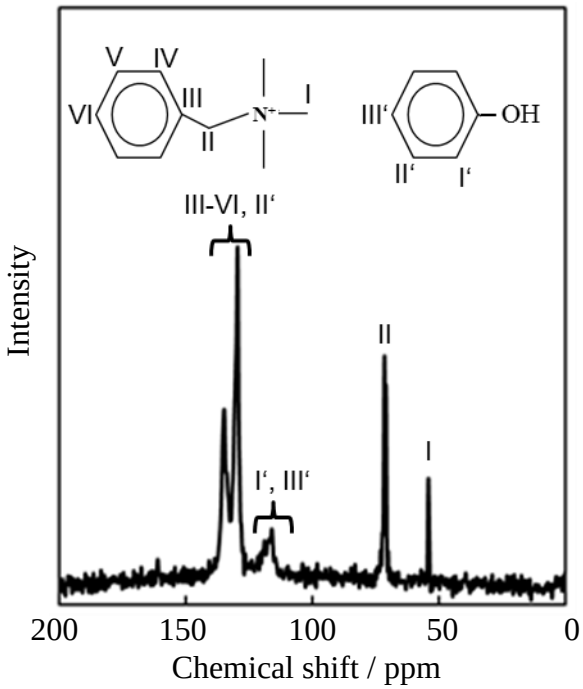

Figure S3 ^{13}C CP-MAS NMR spectrum of HUS-7 after phenol adsorption from acetonitrile.

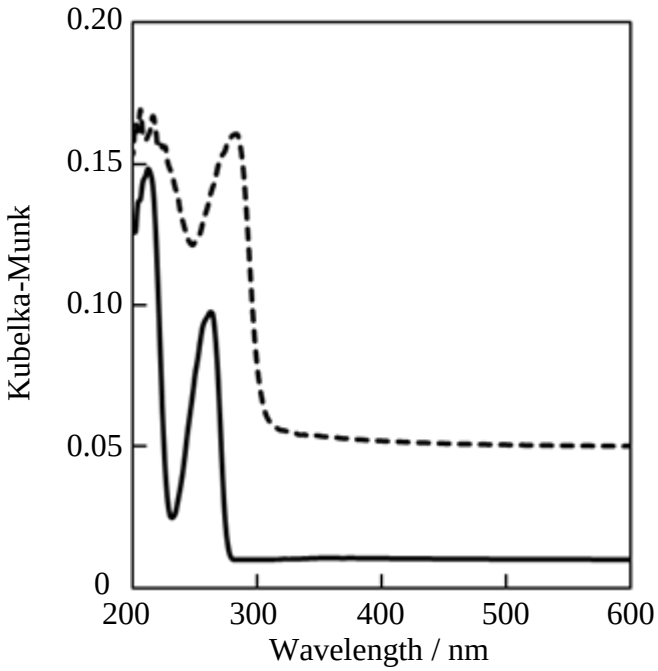

Figure S4 UV-vis spectra of (▬) HUS-7 and (---) HUS-7 after phenol adsorption from acetonitrile.

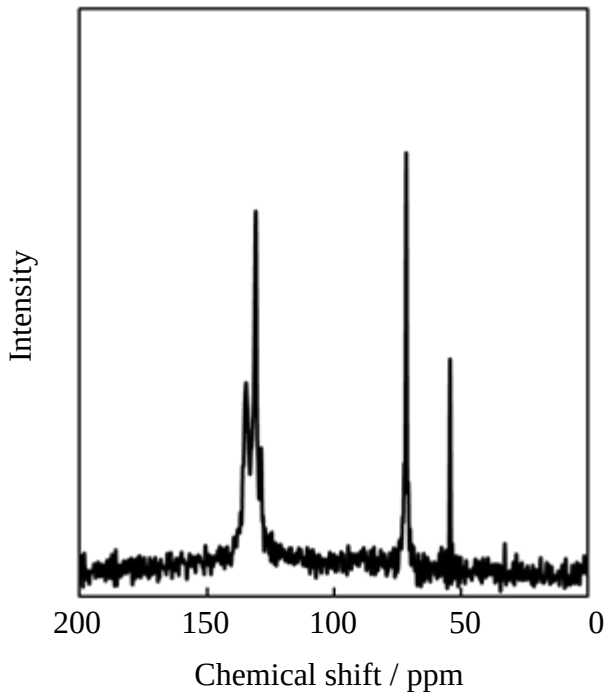

Figure S5 ^{13}C CP-MAS NMR spectrum of HUS-7 after washing with water.

Structure refinement of HUS-7

The initial structure model of HUS-7 was refined by the Rietveld method using the program RIETAN-FP. A split pseudo-Voigt profile function and a background function of Legendre polynomials with 11th order were used in the refinement. Partial profile relaxation with a modified split pseudo-Voigt function was applied to some reflections with highly asymmetric profiles. In the refinement, to enable the solution to converge easily, we imposed restraints upon all the Si–O bond lengths (l(Si–O) = 1.60 ± 0.03 Å) and all the O–Si–O bond angles (ϕ(O–Si–O) = 109.47 ± 5.0°) on geometrical parameters. Likewise, soft restraints were imposed upon all bond lengths and bond angles which were based on the molecular geometry of BTMA. Finally, the atomic coordinates of five Si sites, eleven O sites, ten C sites, one N site, sixteen H sites, and four WO sites were refined. The scattering amplitude of H was added to sites O9 and O11 in terminal silanol groups to maintain the charge balance. All the isotropic atomic displacement parameters, U, for the Si sites were constrained to be equal: U(Si1) = U(Sin: n = 2–5). Simple approximations for U(O1) = U(On: n = 2–11) and B(Cn: n = 1–10) = B(N1) = B(Hn: n = 1–16) were also imposed on the U parameters of the O sites and of the C, N, and H sites, respectively. The U values of all WO sites were fixed at 0.233 Å^{-2} (B = 20 Å^{-2}) for convenience.

Tables S1 and S2 list structural and geometrical parameters obtained by the Rietveld analysis of HUS-7, respectively. The average bond length l(Si–O) and bond angle ϕ(O–Si–O), which were close to expected values, fell within 1.55–1.69 Å and 102.0–117.9°, respectively.

Table S1 Structural parameters *g*, *x*, *y*, *z*, and U_{iso} of HUS-7 obtained by Rietveld refinement. Estimated standard deviations are given as uncertainties in the last reported decimal place

Site	Wycoff	*g*	*x*	*y*	*z*	U_{iso}(Å^2)
Si1	8f	1.0	0.166(1)	0.088(2)	0.0319(5)	0.0197(9)
Si2	8f	1.0	0.4938(9)	0.134(2)	0.0843(5)	= *B*(Si1)
Si3	8f	1.0	0.0890(7)	0.278(2)	0.5033(5)	= *B*(Si1)
Si4	8f	1.0	0.3382(9)	0.100(2)	0.0329(5)	= *B*(Si1)
Si5	8f	1.0	0.0321(9)	0.229(2)	0.0806(5)	= *B*(Si1)
O1	8f	1.0	0.256(2)	0.081(3)	0.0504(9)	0.029(2)
O2	8f	1.0	0.028(2)	0.436(4)	0.0995(9)	= *B*(O1)
O3	8f	1.0	0.354(2)	0.054(4)	0.5015(9)	= *B*(O1)
O4	8f	1.0	0.397(2)	0.114(4)	0.0746(8)	= *B*(O1)
O5	8f	1.0	0.335(2)	0.276(4)	0.0056(9)	= *B*(O1)
O6	8f	1.0	0.025(2)	0.234(4)	0.4633(9)	= *B*(O1)
O7	8f	1.0	0.120(2)	0.165(4)	0.068(1)	= *B*(O1)
O8	8f	1.0	0.530(2)	0.186(3)	0.041(1)	= *B*(O1)
O9	8f	1.0	0.512(1)	0.273(3)	0.1206(9)	= *B*(O1)
O10	8f	1.0	0.149(2)	0.114(3)	0.519(1)	= *B*(O1)
O11	8f	1.0	0.004(2)	0.101(4)	0.1176(8)	= *B*(O1)
N1	8f	1.0	0.228(3)	0.077(5)	0.365(1)	0.008(4)
C1	8f	1.0	0.218(2)	0.268(6)	0.368(2)	= *B*(N1)
C2	8f	1.0	0.171(3)	0.021(7)	0.342(2)	= *B*(N1)
C3	8f	1.0	0.299(3)	0.056(6)	0.348(1)	= *B*(N1)
C4	8f	1.0	0.277(3)	0.479(6)	0.099(2)	= *B*(N1)
C5	8f	1.0	0.226(3)	0.401(6)	0.332(1)	= *B*(N1)
C6	8f	1.0	0.332(3)	0.075(6)	0.220(1)	= *B*(N1)
C7	8f	1.0	0.200(3)	0.102(6)	0.205(2)	= *B*(N1)
C8	8f	1.0	0.164(3)	0.459(6)	0.310(1)	= *B*(N1)
C9	8f	1.0	0.269(3)	0.149(6)	0.229(1)	= *B*(N1)
C10	8f	1.0	0.294(3)	0.479(6)	0.325(2)	= *B*(N1)
H1	8f	1.0	0.27(2)	0.31(5)	0.39(1)	= *B*(N1)
H2	8f	1.0	0.16(2)	0.29(5)	0.38(1)	= *B*(N1)
H3	8f	1.0	0.34(2)	0.14(5)	0.37(1)	= *B*(N1)
H4	8f	1.0	0.30(2)	0.11(5)	0.32(1)	= *B*(N1)
H5	8f	1.0	0.19(2)	0.41(4)	0.15(1)	= *B*(N1)
H6	8f	1.0	0.22(2)	0.47(5)	0.08(1)	= *B*(N1)
H7	8f	1.0	0.18(2)	0.04(5)	0.42(1)	= *B*(N1)
H8	8f	1.0	0.30(2)	0.35(5)	0.11(1)	= *B*(N1)
H9	8f	1.0	0.37(2)	0.47(5)	0.14(1)	= *B*(N1)
H10	8f	1.0	0.31(2)	0.41(6)	0.18(1)	= *B*(N1)
H11	8f	1.0	0.15(2)	0.14(5)	0.32(1)	= *B*(N1)
H12	8f	1.0	0.11(2)	0.40(5)	0.32(1)	= *B*(N1)
H13	8f	1.0	0.35(2)	0.43(5)	0.34(1)	= *B*(N1)
H14	8f	1.0	0.39(2)	0.12(4)	0.24(1)	= *B*(N1)
H15	8f	1.0	0.14(2)	0.16(5)	0.21(1)	= *B*(N1)
H16	8f	1.0	0.27(2)	0.25(5)	0.25(1)	= *B*(N1)
WO1	4e	1.0	0	0.070(8)	0.25	0.233*
WO2	8f	0.85(3)	0.039(4)	0.320(7)	0.196(1)	0.233*
WO3	8f	0.61(5)	0.292(5)	0.49(1)	0.214(2)	0.233*
WO4	8f	1.0	0.264(3)	0.234(6)	0.455(1)	0.233*

*Note: U_{iso} parameters of WO1 and H1 sites were fixed.

Table S2 Selected bond lengths, *l*, and bond angles, ϕ, of HUS-7 obtained by the Rietveld refinement. Estimated standard deviations (ESDs) are given as uncertainties in the last reported decimal digit

l (T–O)	(Å)
Si1– O10	1.55(2)
Si1– O7	1.58(3)
Si1– O5	1.59(3)
Si1– O1	1.60(3)
Si2– O9	1.59(3)
Si2– O2	1.64(3)
Si2– O8	1.66(3)
Si2– O4	1.66(3)
Si3– O3	1.59(3)
Si3– O10	1.65(2)
Si3– O8	1.68(3)
Si3– O6	1.68(3)
Si4– O1	1.57(3)
Si4– O3	1.58(3)
Si4– O5	1.58(3)
Si4– O4	1.64(3)
Si5– O11	1.65(3)
Si5– O7	1.66(3)
Si5– O2	1.66(3)
Si5– O6	1.69(3)
Average	1.627

ϕ (O–T–O)	(°)
O10 – Si1 – O7	116.5(18)
O10 – Si1 – O5	113.3(19)
O10 – Si1 – O1	102.9(17)
O7 – Si1 – O5	112.1(19)
O7 – Si1 – O1	104.4(18)
O5 – Si1 – O1	106.2(17)
O9 – Si2 – O2	107.3(16)
O9 – Si2 – O8	116.2(16)
O9 – Si2 – O4	109.8(16)
O2 – Si2 – O8	109.0(17)
O2 – Si2 – O4	107.9(17)
O8 – Si2 – O4	106.4(16)
O6 – Si3 – O10	103.2(16)
O3 – Si3 – O8	111.2(16)
O3 – Si3 – O6	116.0(18)
O3 – Si3 – O8	106.5(16)
O10 – Si3 – O6	117.2(18)
O10 – Si3 – O6	102.5(14)
O8 – Si4 – O3	112.4(20)
O1 – Si4 – O5	107.1(17)
O1 – Si4 – O4	102.0(19)
O1 – Si4 – O5	102.8(19)
O3 – Si4 – O4	117.9(21)
O3 – Si4 – O4	114.5(18)
O11 – Si5 – O7	110.3(16)
O11 – Si5 – O2	103.3(18)
O11 – Si5 – O6	117.9(18)
O7 – Si5 – O2	115.1(18)
O7 – Si5 – O6	105.2(18)
O2 – Si5 – O6	105.5(18)
Average	109.42