

SSZ-60: a New Large-Pore Zeolite Related to ZSM-23

Supplementary Material

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Fig. 1S. A scanning electron microscopy image of a sample of SSZ-60.

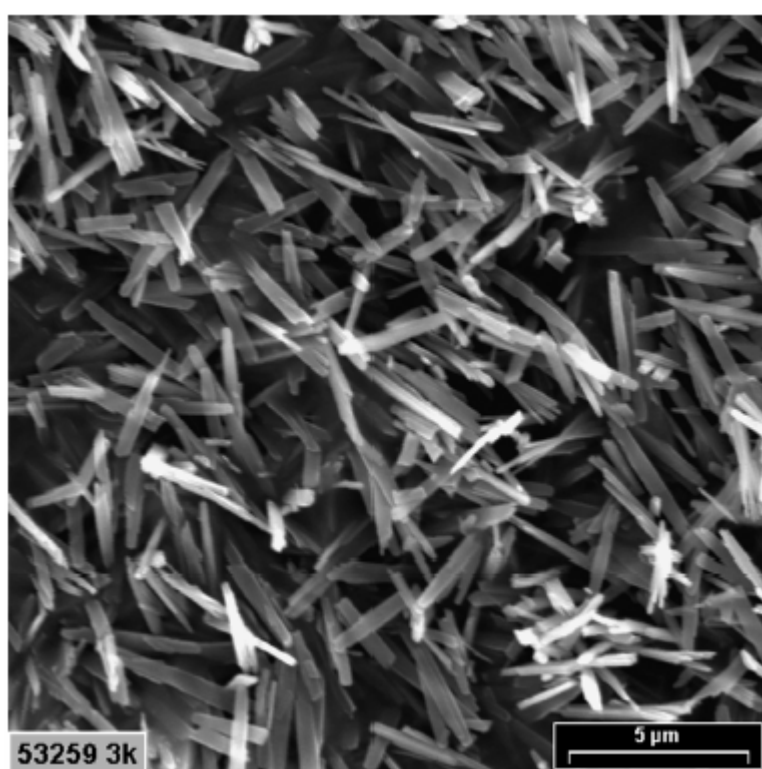


Table 1S. Experimental parameters of synchrotron powder X-ray diffraction experiment for SSZ-60.

Data collection	
X-ray facility	Brookhaven National Laboratory
NSLS beamline	X7A
wavelength	0.7102 Å
temperature	ambient
profile range	2-40° 2θ
step size (°2θ)	0.01
detector	Position sensitive detector
Refinement parameters	
space group	$P2_1nm$
<i>a</i>	5.0122(2) Å
<i>b</i>	13.6985(9) Å
<i>c</i>	21.951(1) Å
background parameters	10
profile parameters	8
R_{wp}	3.33%
R_p	2.55%
R_{wp} background subtracted	5.64%
R_p background subtracted	3.80%
structural parameters	70
$R(F^2)$	0.233
unique reflections	835

Table 2S. Refined atomic parameters of SSZ-60 in space group $P2_1nm$; *a* = 5.0122(2), *b* = 13.6985(9), *c* = 21.951(1) Å.

atom	x	y	z
Si1	0.996(3)	0.1398(9)	1/4
Si2	0.962(2)	0.2195(7)	0.1205(4)
Si3	0.069(2)	0.4046(7)	0.0530(4)
Si4	0.980(2)	0.0805(7)	0.8776(4)
Si5	0.495(3)	0.009(1)	1/4
Si6	0.568(2)	0.3817(7)	0.9700(5)
Si7	0.478(2)	0.1768(7)	0.9256(4)
Si8	0.464(2)	0.1251(7)	0.0655(4)
O1	0.360(3)	0.387(1)	0.0245(6)
O2	0.676(3)	0.120(1)	0.8815(6)
O3	0.543(3)	0.2915(7)	0.9263(7)
O4	0.541(3)	0.4811(6)	0.9278(6)
O5	0.503(4)	0.138(1)	0.9937(4)
O6	0.696(3)	0.098(1)	1/4
O7	0.009(3)	0.3351(8)	0.1075(6)
O8	0.022(3)	0.208(1)	0.1913(3)
O9	0.197(3)	0.052(1)	1/4
O10	0.161(3)	0.156(1)	0.0817(7)
O11	0.510(3)	0.0140(8)	0.0822(7)
O12	0.040(3)	0.058(1)	0.8084(3)
O13	0.660(3)	0.194(1)	0.1032(8)
O14	0.860(3)	0.385(1)	0.9988(6)
O15	0.177(3)	0.1633(9)	0.9019(7)

Table 3S. Coordinates of hypothetical model that may be derived from the MTT structure; in space group $Pmn2_1$; *x* = 26.815, *y* = 11.19, *z* = 4.991 Å.

	x	y	z
O1	0.40387	0.21975	0.34281
O2	0.3309	0.32038	0.60752
O3	0.32579	0.094	0.47691
O4	0.31838	0.25901	0.10767
O5	0.44181	0.35749	0.97211
O6	0.44187	0.42682	0.47198
O7	0.24073	0.02849	0.26858
O8	0.09644	0.44494	0.34087
O9	0.3151	0.48468	0.97138
O10	0.5	0.2525	0.31947
O11	0	0.47641	0.31947
O12	0.17606	0.32314	0.20835
O13	0.14846	0.33458	0.70821
O14	0.24312	0.34042	0.83046
O15	0.19294	0.14196	0.88914
Si1	0.1514	0.40708	0.43183
Si2	0.44689	0.3139	0.27659
Si3	0.44673	0.47023	0.77689
Si4	0.30202	0.35133	0.87916
Si5	0.19006	0.28463	0.90881
Si6	0.21708	0.01663	0.97542
Si7	0.34469	0.22329	0.38405

Table 4Sa. Atomic distances and Si-O-Si angles of SSZ-60 framework atoms.

Si-O distances (Å)				T-O-T Angles (°)	
Si1-O6	1.611	Si7-O2	1.587	Si3-O1-Si6	154
Si1-O8	1.592	Si7-O3	1.605	Si4-O2-Si7	142
Si1-O8	1.592	Si7-O5	1.592	Si6-O3-Si7	142
Si1-O9	1.574	Si7-O15	1.607	Si3-O4-Si6	130
<Si1-O>	1.592	<Si7-O>	1.598	Si7-O5-Si8	162
				Si1-O6-Si5	151
Si2-O7	1.627	Si8-O5	1.597	Si2-O7-Si3	139
Si2-O8	1.593	Si8-O10	1.616	Si1-O8-Si2	147
Si2-O10	1.579	Si8-O11	1.581	Si1-O9-Si5	151
Si2-O13	1.596	Si8-O13	1.591	Si2-O10-Si8	149
<Si2-O>	1.599	<Si8-O>	1.596	Si4-O11-Si8	155
				Si4-O12-Si5	149
Si3-O1	1.607			Si2-O13-Si8	147
Si3-O4	1.627			Si3-O14-Si6	154
Si3-O7	1.557			Si4-O15-Si7	141
Si3-O14	1.608			<Si-O-Si>	148
<Si3-O>	1.600				
Si4-O2	1.620				
Si4-O11	1.575				
Si4-O12	1.579				
Si4-O15	1.597				
<Si4-O>	1.593				
Si5-O6	1.577				
Si5-O9	1.602				
Si5-O12	1.594				
Si5-O12	1.594				
<Si5-O>	1.592				
Si6-O1	1.587				
Si6-O3	1.571				
Si6-O4	1.653				
Si6-O14	1.595				
<Si6-O>	1.602				

Table 4Sb. Tetrahedral angles of framework atoms in SSZ-60.

Tetrahedral Angles (°)			
O6-Si1-O8	106.5	O2-Si7-O3	110.8
O6-Si1-O8	106.5	O2-Si7-O5	111.0
O6-Si1-O9	108.8	O2-Si7-O15	109.5
O8-Si1-O8	108.0	O3-Si7-O5	107.7
O8-Si1-O9	113.3	O3-Si7-O15	107.9
O8-Si1-O9	113.3	O5-Si7-O15	109.9
<O-Si1-O>	109.4	<O-Si7-O>	109.5
O7-Si2-O8	104.1	O5-Si8-O10	107.8
O7-Si2-O10	110.7	O5-Si8-O11	108.4
O7-Si2-O13	108.3	O5-Si8-O13	111.9
O8-Si2-O10	110.4	O10-Si8-O11	109.5
O8-Si2-O13	112.9	O10-Si8-O13	108.3
O10-Si2-O13	110.3	O11-Si8-O13	110.9
<O-Si2-O>	109.5	<O-Si8-O>	109.5
O1-Si3-O4	109.1		
O1-Si3-O7	112.4		
O1-Si3-O14	106.0		
O4-Si3-O7	111.9		
O4-Si3-O14	107.1		
O7-Si3-O14	110.1		
<O-Si3-O>	109.4		
O2-Si4-O11	109.8		
O2-Si4-O12	107.4		
O2-Si4-O15	109.0		
O11-Si4-O12	111.2		
O11-Si4-O15	109.6		
O12-Si4-O15	109.9		
<O-Si4-O>	109.5		
O6-Si5-O9	108.5		
O6-Si5-O12	110.7		
O6-Si5-O12	110.7		
O9-Si5-O12	110.0		
O9-Si5-O12	110.0		
O12-Si5-O12	106.9		
<O-Si5-O>	109.5		
O1-Si6-O3	116.1		
O1-Si6-O4	109.5		
O1-Si6-O14	107.7		
O3-Si6-O4	107.4		
O3-Si6-O14	109.9		
O4-Si6-O14	105.7		
<O-Si6-O>	109.4		