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Assessment of ordered and complementary pore volumes in polymer-templated mesoporous silicas and organosilicas

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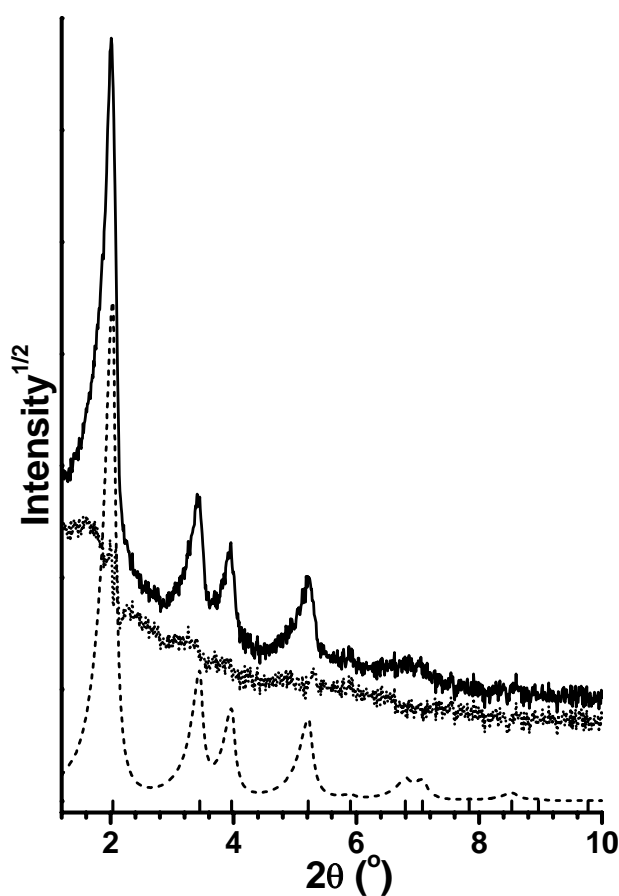[b]Institute of Chemistry and Chemical Technology, 660049 Krasnoyarsk, Russia

Figure S1. Weighted observed (solid line), calculated (dashed line), and difference (dotted line) XRD patterns for the MCM-41-C18 sample after DDM full-profile structure refinement. The calculated diffraction reflection positions are marked by inward ticks. Details about XRD measurements are reported in *Microporous Mesoporous Mater*., **2001**, *48*, 127.

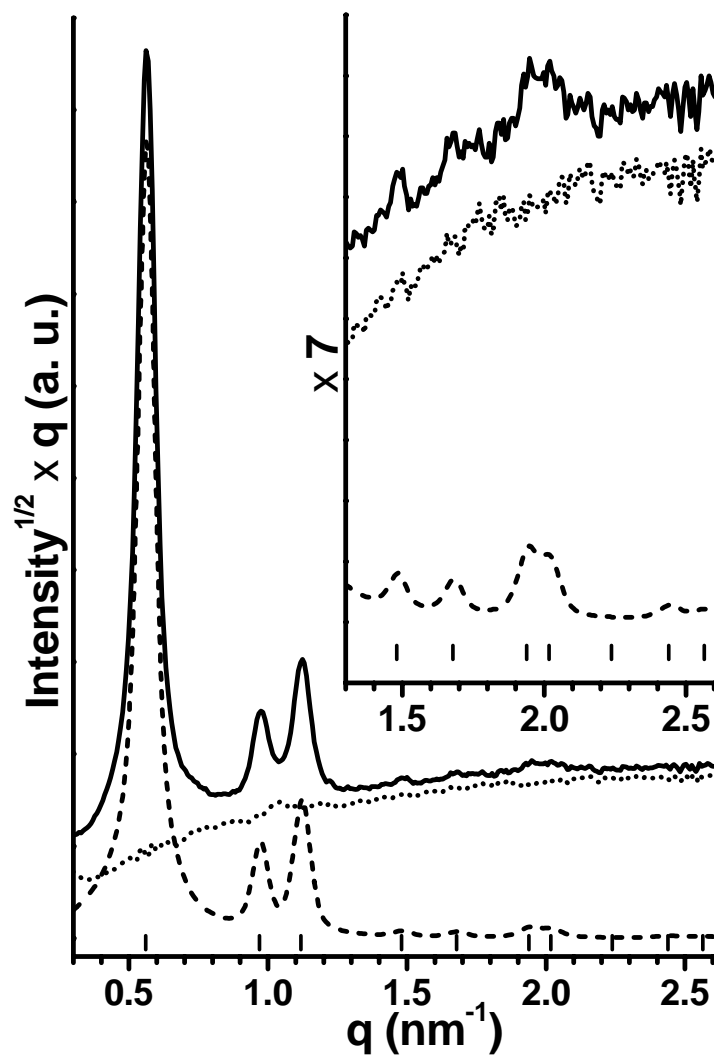* Tel. (330) 672 3790; Fax (330) 672 3816; E-mail: jaroniec@kent.edu

Figure S2. Weighted and Lorentz-corrected observed (solid line), calculated (dashed line), and difference (dotted line) SAXS patterns for the SBA15 silica containing ethane bridging groups (SBA-15-E) after DDM full-profile structure refinement. The calculated diffraction reflection positions are marked by ticks. Details about SAXS measurements are reported in *J. Phys. Chem. B,* **2006**, *110*, 2972.
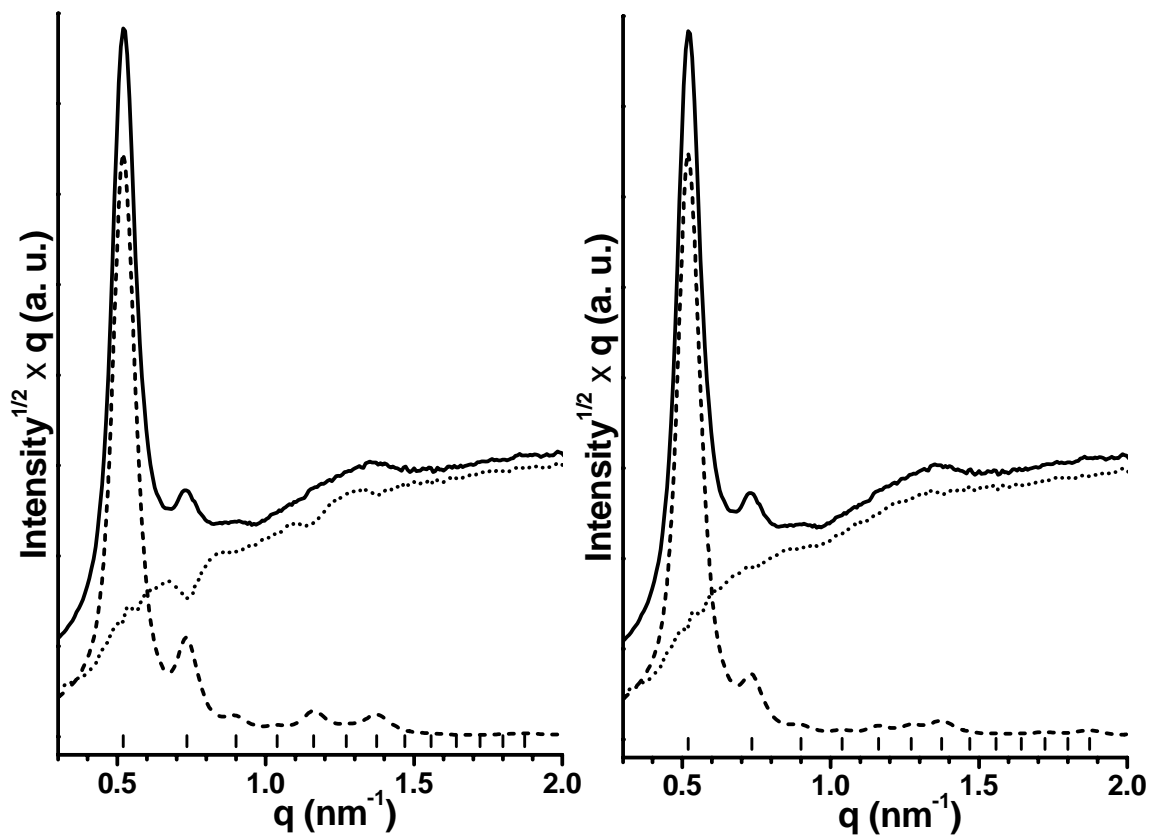
Figure S3. Weighted and Lorentz-corrected observed (solid line), calculated (dashed line), and difference (dotted line) SAXS patterns for SBA16-ICS sample after DDM structure refinement (left) and DDM pattern decomposition (right). The calculated diffraction reflection positions are marked by ticks. Details about SAXS measurements are reported in *Chem. Mater.,* **2006**, *18*, in press.

Table S1. Structural parameters for the SBA-15 samples obtained by DDM. [a]

Sample	a, nm	w, nm	t, nm	Hex, %	B, nm^2
SBA-15/06	11.66	8.63	3.02	27.1	29.1
SBA-15/24	12.12	9.39	2.74	26.9	40.4
SBA-15/72	12.43	10.02	2.41	28.4	43.3
SBA-15/96	12.45	10.10	2.35	20.0	41.1
SBA-15/12*	12.29	9.72	2.56	28.0	42.7
SBA-15/48*	11.98	9.87	2.11	9.0	47.2
SBA-15/72*	12.44	10.37	2.07	11.1	46.3
SBA-15-E	12.97	9.00	3.96	19.6	29.1

[a] a, the lattice parameter; w, the pore size; t, the wall thickness ($t = a - w$); Hex, the pore shape hexagonality; B, the isotropic displacement parameter in the Debye-Waller factor.
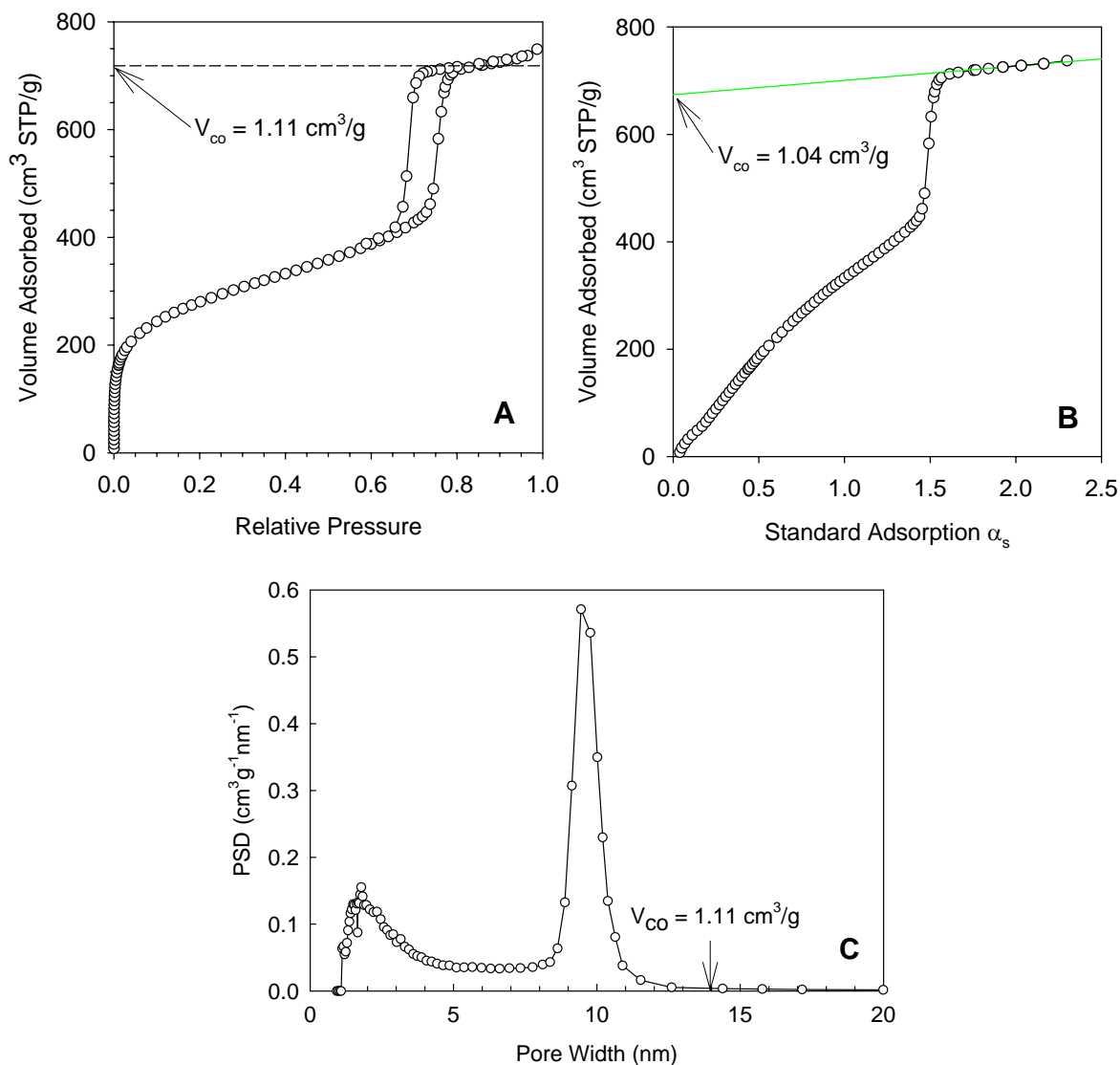
Figure S4. Illustration of three methods for estimating the pore volume V_{co}, which includes the volume of ordered mesopores as well as the volume of complementary pores (i.e., micropores present in the mesopore walls and in the case of cage-like materials, interconnecting ordered apertures between neighboring ordered cages) from nitrogen adsorption data for SBA-15/06. **Panel A** shows the estimation of V_{co} directly from nitrogen adsorption isotherm by converting the amount adsorbed at the isotherm plateau, which appears after steep step reflecting capillary condensation in ordered mesopores, to the volume of liquid adsorbate; **Panel B** shows the evaluation of this pore volume by converting the intercept of the linear segment of the α_s-plot that appears after capillary condensation step, to the volume of liquid adsorbate, and **Panel C** illustrates the estimation of this volume by integration of the differential pore size distribution (in this case PSD was obtained by the KJS method) over the pore range including complementary small pores and ordered mesopores.
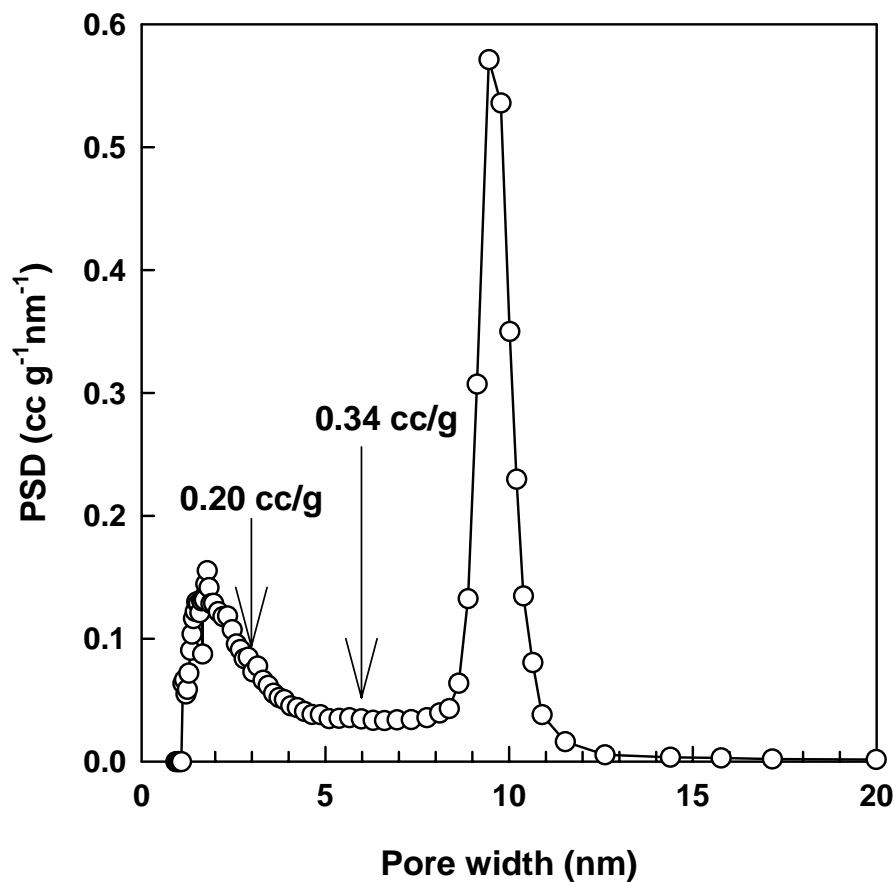
Figure S5. Differential pore size distribution (PSD) calculated by the KJS method for SBA-15/06; integration of PSD up to 3nm gives the pore volume of 0.20 cc/g, whereas integration up to 6.5 nm gives the value of 0.36 cc/g.